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Thermodynamic Properties of Halides

By L. B. Pankratz

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Thermodynamic data on the halides were reviewed, evaluated, and compiled at the Bureau of Mines Albany Research Center. The values for heat capacities, high-temperature relative enthalpies, enthalpies of formation, and Gibbs energies of formation are given in both tabular and equation forms. The tables include entropy, Gibbs energy functions, and logarithms (base 10) of the equilibrium constants. Where possible, all phases of a halide are presented in a single table. Temperatures of transformation and thermodynamic properties at these temperatures are included in the table. Immediately below the table the natures of transformations are given along with their associated enthalpies.

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THERMODYNAMIC PROPERTIES OF HALIDES

By L. B. Pankratz[1]

ABSTRACT

Thermodynamic data on the halides were reviewed, evaluated, and compiled at the Bureau of Mines Albany Research Center. Values for $C_p°$, $S°$, $H°-H°_{298}$, $-(G°-H°_{298})/T$, $\Delta Hf°$, $\Delta Gf°$, and log Kf are given in tabular form. $C_p°$, $H°-H°_{298}$, $\Delta Hf°$, and $\Delta Gf°$ are also expressed algebraically.

INTRODUCTION

This compilation is the second in a series revising and expanding Bureau of Mines Bulletin 605, "Thermodynamic Properties of 65 Elements—Their Oxides, Halides, Carbides, and Nitrides," by C. E. Wicks and F. E. Block, published in 1963, and including data available through 1959. The first volume in the present series, Bureau of Mines Bulletin 672, "Thermodynamic Properties of Elements and Oxides," by L. B. Pankratz (*184*),[2] was published in 1982. These works are part of the Bureau of Mines continuing effort to provide information for use as guidelines in mineral technology advancement, pollution control, and energy economy.

Wicks and Block prepared their bulletin ". . . to encourage the application of thermodynamics in the metallurgical field; consequently, the values have been presented in a simple, readily usable form." This compilation has been prepared in the same spirit. The values for heat capacities, $C_p°$; high-temperature relative enthalpies, $H°-H°_{298}$; enthalpies of formation, $\Delta Hf°$; and Gibbs energies of formation, $\Delta Gf°$ are given in both tabular and equation forms. The tables include entropy, $S°$; Gibbs energy functions, $-(G°-H°_{298})/T$; and logarithms (base 10) of the equilibrium constants, log Kf. For the halides of sulfur, selenium, and tellurium only, the values for ΔH, ΔG, and log K were calculated using $S_2(g)$, $Se_2(g)$, and $Te_2(g)$. Since these are not standard state formation reactions, the symbols ΔHf, ΔGf, and log Kf have been replaced with ΔHr, ΔGr, and log Kr.

Where possible, all phases of a halide are presented in a single table. Temperatures of transformation and thermodynamic properties at these temperatures are included in the table. Immediately below the table the natures of transformations are given along with their associated enthalpies.

Bulletin 672 contains a section, "Process Applications," giving a short statement of some fundamental ideas of thermodynamics and includes several examples of their use. These examples illustrate several alternate methods of calculation using both the tabulated values and the equations. Comparisons are also made on the bases of ease of calculation and accuracy of results.

[1] Research chemist, Albany Research Center, Bureau of Mines, Albany, OR.

[2] Italicized and/or underlined numbers in parentheses refer to items in the list of references at the end of this Bulletin.

METHODS, CONVENTIONS, AND SYMBOLS

The values in this compilation are the result of a review and critical evaluation of relevant thermodynamic data through 1981 for the halides. Some data published in 1982 have been included. Data for the elements used in this compilation are from Bulletin 672. Generally, unless more recent and reliable data were available, the values for the standard enthalpy of formation at 298.15 K were taken from the NBS Technical Note 270 series. The values for many gases were taken from the JANAF Thermochemical Tables. Specific references are made to these publications where they are used.

The selected experimental data were fit with a polynomial in terms of temperature by using a modified form of the computer program described by Justice (*112*). This program, along with a plot of the function $(H°–H°_{298})/(T–298.15)$, which must take the value of $C_p°$ at 298.15 K, was used to merge smoothly high-temperature data with low-temperature heat capacity data. The resulting polynomial was then used in a subroutine of the program to calculate standard heat capacities, relative enthalpies, Gibbs energy functions, and entropies at selected temperatures. These values are also tabulated at transformation temperatures. In addition, the tables include values for the standard enthalpy of formation, the Gibbs energy of formation, and the logarithm of the equilibrium constant of formation.

Tabulated values and the equations are for the substances in their standard states (indicated by the superscript °). Standard states for the pure condensed substances are the most stable form at 1 atm pressure at the specified temperature. For vitreous and metastable substances the superscript refers to the pure substance. For gases, the standard state is the pure substance as a hypothetical ideal gas at unit fugacity.

Tabular values of relative enthalpies are represented by algebraic equations in the form recommended by Maier and Kelley (*152*). This form was fit to the data by Kelley's method (*117*). *Since they consist of no more than four terms, they give less precise values than the tabular values.* However, they do furnish a convenient means of representation. These equations are given below each table. A separate equation is given whenever a transformation occurs. In some cases two equations are used to represent a single phase with an extended temperature range, for example, HCl(*g*) and HF(*g*), since a single equation would give unacceptable errors.

The equations for standard heat capacity, enthalpy of formation, and Gibbs energy of formation are also given below the tables. Since these equations were derived using the equations for standard relative enthalpies, they too give less precise values than the tabular values. Examples in the "Process Applications" section of Bulletin 672 show the methods of derivation.

Sources of data used in this compilation are given in the references section, which is not meant to be exhaustive. For simplicity, additional sources reviewed and considered less reliable were not included. Estimates were used where the necessary data were lacking. Estimated and extrapolated values are indicated in the tables with an asterisk (*) and a note immediately below the table. An asterisk and a note are used to indicate decomposition, metastable phases, and irreversible transformations.

The common practice of tabulating five- and sometimes six-digit values has been followed. For example, enthalpy values are given to the nearest calorie. The number of digits given is not intended to reflect the accuracy of the experimental values used. It is an effort to produce internal consistency in the tabulated values.

The following is a list of symbols and constants used:

°	Standard state.
T	Thermodynamic temperature in kelvins.
K	Kelvin, the unit of thermodynamic temperature.
C_p	Heat capacity at constant pressure.
S	Entropy.
$H–H_{298}$	Enthalpy increment between T and 298.15 K.
$(G–H_{298})/T$	Gibbs energy function, $[(H–H_{298})/T]–S$.
ΔH	Enthalpy change (ΔHf = enthalpy of formation).
ΔG	Gibbs energy change (ΔGf = Gibbs energy of formation).
log K	Logarithm (base 10) of the equilibrium constant (log Kf = equilibrium constant of formation).
cal	Thermochemical calorie, 1 cal = 4.1840 J.
mol	Molar mass.
ln	Natural logarithm, base e = 2.7183.
P	Pressure in atmospheres, 1 atm = 101.325 kPa.
R	Gas constant, 1.98719 cal/mol · K.
F	Faraday constant, 23060.9 cal/V equivalent.

THERMODYNAMIC DATA FOR HALIDES

In the following pages, thermodynamic values for the halides are given in both tabular and equation forms. The tables have the base temperature 298.15 K, and are not extended much above the temperature of the available data. Except in tables or equations, the base temperature is usually abbreviated as 298 K. To avoid confusion, the standard state at this base temperature is indicated in each table heading and in the chemical formation equation. The symbols *c*, *l*, *g*, and *vit* refer respectively to crystal, liquid, gas, and vitreous phases. Also, the Greek letters α, β, γ, δ, and ε are used to denote different crystalline forms. In a few instances, Greek letters also denote substances above and below a second-order transformation. Again, to avoid confusion, where substances have the same chemical formula but different standard states, the standard state is explicitly given in the heading; for example, BeF_2 (c, *l*) and BeF_2 (vitreous).

Many of the experimental measurements of thermodynamic properties used in this compilation were obtained using the International Practical Temperature Scale of 1948 (IPTS—48). This scale has been superseded by IPTS—68 (*35*) and the amended edition of 1975 (*36*). These scales differ by as much as 2.6 K (at 2000 K), but no attempt has been made, except as specifically noted, to convert earlier measurements to IPTS—68 since the errors involved are less than experimental errors.

The tables are arranged in alphabetical order by chemical symbols. For convenience, the chemical symbol of the pertinent element has been included in pagination.

AgBr(c,l)
Silver Bromide
[Formation: $Ag(c) + 0.5Br_2(l,g) = AgBr(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	13.050	25.600	25.600	0	-24.038	-23.215	17.017
300	13.060	25.680	25.600	.024	-24.042	-23.209	16.908
332.6	13.278	27.039	25.676	.453	-24.105	-23.116	15.189
332.6	13.278	27.039	25.676	.453	-27.637	-23.116	15.189
400	13.730	29.520	26.120	1.360	-27.438	-22.221	12.141
500	14.740	32.680	27.120	2.780	-27.083	-20.954	9.159
600	17.680	35.560	28.285	4.365	-26.576	-19.768	7.201
700	30.400	39.060	29.560	6.650	-25.389	-18.712	5.842
700	14.460	41.960	29.560	8.680	-23.359	-18.712	5.842
800	14.360	43.890	31.234	10.125	-23.030	-18.072	4.937
900	14.220	45.570	32.737	11.550	-22.739	-17.473	4.243
1000	14.060	47.060	34.095	12.965	-22.475	-16.901	3.694
1100	13.920	48.400	35.341	14.365	-22.247	-16.360	3.250
1200	13.780	49.600	36.471	15.755	-22.051	-15.822	2.882

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
700 K, melting point of AgBr; ΔH° = 2.030 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp^\circ = -8.746 + 43.038\times10^{-3}T + 7.960\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = -8.746\times10^{-3}T + 21.519\times10^{-6}T^2 - 7.960\times10^{2}T^{-1} + 3.365$

700-1200 K: $Cp^\circ = 15.300 - 1.200\times10^{-3}T$

$H^\circ - H^\circ_{298} = 15.300\times10^{-3}T - 0.600\times10^{-6}T^2 - 1.736$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -16.402 - 23.063\times10^{-3}T + 20.651\times10^{-6}T^2 - 773.800T^{-1}$

$\Delta Gf^\circ = -16.402 + 23.063\times10^{-3}T\ln T - 20.651\times10^{-6}T^2 - 386.900T^{-1} - 143.749\times10^{-3}T$

332.6-700 K: $\Delta Hf^\circ = -21.402 - 18.483\times10^{-3}T + 20.573\times10^{-6}T^2 - 789.500T^{-1}$

$\Delta Gf^\circ = -21.402 + 18.483\times10^{-3}T\ln T - 20.573\times10^{-6}T^2 - 394.750T^{-1} - 102.071\times10^{-3}T$

700-1200 K: $\Delta Hf^\circ = -26.503 + 5.563\times10^{-3}T - 1.546\times10^{-6}T^2 + 6.500T^{-1}$

$\Delta Gf^\circ = -26.503 - 5.563\times10^{-3}T\ln T + 1.546\times10^{-6}T^2 + 3.250T^{-1} + 46.448\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Parker (188). Other data from Pankratz (183).

AgCl(c,l)
Silver Chloride
[Formation: $Ag(c,l) + 0.5Cl_2(g) = AgCl(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	12.640	23.000	23.000	0	-30.370	-26.251	19.242
300	12.660	23.080	23.003	.023	-30.365	-26.226	19.105
400	13.250	26.800	23.500	1.320	-30.096	-24.885	13.596
500	13.890	29.820	24.470	2.675	-29.790	-23.615	10.322
600	14.740	32.420	25.587	4.100	-29.434	-22.414	8.164
700	17.080	34.840	26.740	5.670	-28.955	-21.282	6.644
730	20.160	35.600	27.084	6.215	-28.740	-20.954	6.273
730	14.630	39.630	27.084	9.160	-25.795	-20.954	6.273
800	14.460	40.960	28.235	10.180	-25.556	-20.497	5.599
900	14.230	42.660	29.754	11.615	-25.251	-19.893	4.831
1000	14.030	44.140	31.115	13.025	-24.989	-19.307	4.219
1100	13.830	45.470	32.361	14.420	-24.763	-18.749	3.725
1200	13.630	46.660	33.502	15.790	-24.585	-18.208	3.316
1235.08	13.560	47.052	33.881	16.267	-24.532	-18.018	3.188
1235.08	13.560	47.052	33.881	16.267	-27.232	-18.018	3.188
1300	13.430	47.750	34.562	17.145	-27.166	-17.542	2.949
1400	13.230	48.740	35.540	18.480	-27.083	-16.806	2.623

Phase changes: 730 K, melting point of AgCl; $\Delta H°$ = 2.945 kcal/mol.
1235.08 K, melting point of Ag; $\Delta H°$ = 2.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-730 K: $Cp° = 7.194 + 12.658\times10^{-3}T + 1.500\times10^{5}T^{-2}$
$H°- H°_{298} = 7.194\times10^{-3}T + 6.329\times10^{-6}T^{2} - 1.500\times10^{2}T^{-1} - 2.204$

730-1400 K: $Cp° = 16.170 - 2.120\times10^{-3}T$
$H°- H°_{298} = 16.170\times10^{-3}T - 1.060\times10^{-6}T^{2} - 2.079$

Formation equations (kcal/mol):

298.15-730 K: $\Delta Hf° = -29.561 - 2.491\times10^{-3}T + 5.367\times10^{-6}T2 - 161.950T^{-1}$
$\Delta Gf° = -29.561 + 2.491\times10^{-3}T\ln T - 5.367\times10^{-6}T^{2} - 80.975T^{-1} - 0.583\times10^{-3}T$

730-1235.08 K: $\Delta Hf° = -29.436 + 6.485\times10^{-3}T - 2.022\times10^{-6}T^{2} - 11.950T^{-1}$
$\Delta Gf° = -29.436 - 6.485\times10^{-3}T\ln T + 2.022\times10-6T^{2} - 5.975T^{-1} + 52.891\times10^{-3}T$

1235.08-1400 K: $\Delta Hf° = -30.149 + 3.756\times10^{-3}T - 1.104\times10^{-6}T^{2} - 34.150T^{-1}$
$\Delta Gf° = -30.149 - 3.756\times10^{-3}T\ln T + 1.104\times10^{-6}T^{2} - 17.075T^{-1} + 35.189\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from CODATA (188). Other data from Pankratz (183).

AgI(c,l)
Silver Iodide
[Formation: $Ag(c) + 0.5I_2(c,l,g) = AgI(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	13.580	27.600	27.600	0	-14.780	-15.839	11.610
300	13.599	27.684	27.601	.025	-14.778	-15.845	11.543
386.8	14.727	31.252	28.032	1.245	-14.692	-16.166	9.134
386.8	14.727	31.252	28.032	1.245	-16.547	-16.166	9.134
400	14.898	31.749	28.147	1.441	-16.560	-16.153	8.826
421	15.661	32.528	28.348	1.760	-16.573	-16.132	8.374
421	13.982	36.020	28.348	3.230	-15.103	-16.132	8.374
458.4	13.830	37.204	29.023	3.750	-15.176	-16.219	7.733
458.4	13.830	37.204	29.023	3.750	-20.186	-16.219	7.733
500	13.660	38.392	29.752	4.320	-20.063	-15.863	6.934
600	13.589	40.873	31.405	5.681	-19.786	-15.048	5.481
700	13.622	42.970	32.911	7.041	-19.526	-14.280	4.458
800	13.890	44.801	34.285	8.413	-19.272	-13.547	3.701
831	14.100	45.332	34.688	8.845	-19.191	-13.328	3.505
831*	14.000	48.040	34.688	11.095	-16.941	-13.328	3.505
900	14.000	49.157	35.756	12.061	-16.762	-13.038	3.166
1000	14.000	50.632	37.171	13.461	-16.515	-12.637	2.762
1100	14.000	51.967	38.457	14.861	-16.290	-12.260	2.436
1200	14.000	53.185	39.634	16.261	-16.086	-11.903	2.168

*Data for liquid estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
421 K, transition point of AgI; ΔH° = 1.470 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
831 K, melting point of AgI; ΔH° = 2.250 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-421 K: $Cp^\circ = 0.337 + 31.064\times10^{-3}T + 3.539\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 0.337\times10^{-3}T + 15.532\times10^{-6}T^2 - 3.539\times10^{2}T^{-1} - 0.294$

421-831 K: $Cp^\circ = 10.436 + 3.544\times10^{-3}T + 3.640\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 10.436\times10^{-3}T + 1.772\times10^{-6}T^2 - 3.640\times10^{2}T^{-1} - 0.613$

831-1200 K: $Cp^\circ = 14.000$

$H^\circ - H^\circ_{298} = 14.000\times10^{-3}T - 0.539$

AgI(c,l) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -11.509 - 11.373\times10^{-3}T + 13.868\times10^{-6}T^2 - 331.700T^{-1}$

$\Delta Gf^\circ = -11.509 + 11.373\times10^{-3}T\ln T - 13.868\times10^{-6}T^2 - 165.850T^{-1} - 73.322\times10^{-3}T$

386.8-421 K: $\Delta Hf^\circ = -12.237 - 14.576\times10^{-3}T + 14.614\times10^{-6}T^2 - 331.700T^{-1}$

$\Delta Gf^\circ = -12.237 + 14.576\times10^{-3}T\ln T - 14.614\times10^{-6}T^2 - 165.850T^{-1} - 90.230\times10^{-3}T$

421-458.4 K: $\Delta Hf^\circ = -12.556 - 4.476\times10^{-3}T + 0.854\times10^{-6}T2 - 341.800T^{-1}$

$\Delta Gf^\circ = -12.556 + 4.476\times10^{-3}T\ln T - 0.854\times10^{-6}T^2 - 170.900T^{-1} - 34.213\times10^{-3}T$

458.4-831 K: $\Delta Hf^\circ = -19.912 + 0.694\times10^{-3}T + 0.820\times10^{-6}T^2 - 349.450T^{-1}$

$\Delta Gf^\circ = -19.912 - 0.694\times10^{-3}T\ln T - 0.820\times10^{-6}T^2 - 174.725T^{-1} + 13.519\times10^{-3}T$

831-1200 K: $\Delta Hf^\circ = -19.838 + 4.258\times10^{-3}T - 0.952\times10^{-6}T^2 + 14.550T^{-1}$

$\Delta Gf^\circ = -19.838 - 4.258\times10^{-3}T\ln T + 0.952\times10^{-6}T^2 + 7.275T^{-1} + 35.653\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (253). Low-temperature heat capacities and entropy at 298 K from Pitzer (195). Data from 298 K to 831 K based on Noelting (172). Enthalpy of fusion from Kelley (116). Heat capacity of liquid estimated.

AlBr(g)
Aluminum Monobromide (ideal gas)
[Formation: $Al(c,l) + 0.5Br_2(l,g) = AlBr(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.509	57.244	57.244	0	3.800	-5.824	4.269
300	8.514	57.296	57.244	.016	3.789	-5.883	4.286
332.6	8.578	58.178	57.292	.295	3.581	-6.923	4.549
332.6	8.578	58.178	57.292	.295	.049	-6.923	4.549
400	8.710	59.776	57.581	.878	-.069	-8.328	4.550
500	8.816	61.732	58.222	1.755	-.257	-10.370	4.533
600	8.882	63.345	58.945	2.640	-.466	-12.372	4.507
700	8.927	64.718	59.674	3.531	-.704	-14.338	4.476
800	8.961	65.912	60.381	4.425	-.976	-16.268	4.444
900	8.988	66.969	61.056	5.322	-1.289	-18.162	4.410
933.61	8.996	67.299	61.275	5.624	-1.403	-18.790	4.399
933.61	8.996	67.299	61.275	5.624	-3.983	-18.790	4.399
1000	9.011	67.918	61.696	6.222	-4.189	-19.837	4.335
1100	9.030	68.777	62.300	7.125	-4.496	-21.385	4.249
1200	9.048	69.564	62.874	8.028	-4.804	-22.908	4.172
1300	9.065	70.289	63.417	8.934	-5.109	-24.405	4.103
1400	9.080	70.961	63.932	9.841	-5.414	-25.876	4.039
1500	9.095	71.588	64.421	10.750	-5.718	-27.328	3.982
1600	9.109	72.176	64.889	11.660	-6.022	-28.760	3.928
1700	9.123	72.728	65.333	12.572	-6.324	-30.171	3.879
1800	9.137	73.250	65.758	13.485	-6.625	-31.565	3.832
1900	9.150	73.744	66.166	14.399	-6.926	-32.940	3.789
2000	9.163	74.214	66.556	15.315	-7.226	-34.303	3.748

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.901 + 0.142\times10^{-3}T - 0.387\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.901\times10^{-3}T + 0.071\times10^{-6}T^2 + 0.387\times10^{2}T^{-1} - 2.790$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = 5.167 - 4.736\times10^{-3}T - 1.606\times10^{-6}T^2 + 56.100T^{-1}$

$\Delta Gf^\circ = 5.167 + 4.736\times10^{-3}T\ln T + 1.606\times10^{-6}T^2 + 28.050T^{-1} - 64.644\times10^{-3}T$

332.6-933.61 K: $\Delta Hf^\circ = 0.167 - 0.156\times10^{-3}T - 1.684\times10^{-6}T^2 + 40.400T^{-1}$

$\Delta Gf^\circ = 0.167 + 0.156\times10^{-3}T\ln T + 1.684\times10^{-6}T^2 + 20.200T^{-1} - 22.966\times10^{-3}T$

933.61-2000 K: $\Delta Hf^\circ = -1.101 - 3.154\times10^{-3}T + 0.044\times10^{-6}T^2 + 23.000T^{-1}$

$\Delta Gf^\circ = -1.101 + 3.154\times10^{-3}T\ln T - 0.044\times10^{-6}T^2 + 11.500T^{-1} - 40.490\times10^{-3}T$

Source: Data from JANAF (63).

$AlBr_3(c,l)$
Aluminum Tribromide
[Formation: $Al(c) + 1.5Br_2(l,g) = AlBr_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	24.040	43.080	43.080	0	-122.160	-116.714	85.553
300	24.100	43.220	43.080	.050	-122.171	-116.672	84.994
332.6	25.293	45.774	43.205	.854	-122.440	-116.064	76.264
332.6	25.293	45.774	43.205	.854	-133.037	-116.064	76.264
350	25.930	47.080	43.366	1.300	-132.923	-115.179	71.920
370.6	27.030	48.590	43.626	1.840	-132.777	-114.148	67.314
370.6	29.870	55.850	43.626	4.530	-130.087	-114.148	67.314
400	29.870	58.130	44.605	5.410	-129.772	-112.893	61.681
500	29.870	64.800	48.000	8.400	-128.729	-108.795	47.553
529	29.870	66.480	48.975	9.260	-128.440	-107.651	44.474

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
370.6 K, melting point of $AlBr_3$; $\Delta H°$ = 2.690 kcal/mol.
529 K, boiling point to $(AlBr_3)_2(g)$. $\Delta H°$(sublimation, 298 K) = 20.4 kcal/mol of dimer.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-370.6 K: $Cp° = 31.876 - 1.952\times10^{-3}T - 6.441\times10^{5}T^{-2}$
$H°- H°_{298} = 31.876\times10^{-3}T - 0.976\times10^{-6}T^2 + 6.441\times10^{2}T^{-1} - 11.577$

370.6-529 K: $Cp° = 29.870$
$H°- H°_{298} = 29.870\times10^{-3}T - 6.540$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -124.196 + 0.147\times10^{-3}T - 2.553\times10^{-6}T^2 + 661.500T^{-1}$
$\Delta Gf° = -124.196 - 0.147\times10^{-3}T\ln T + 2.553\times10^{-6}T^2 + 330.750T^{-1} + 21.451\times10^{-3}T$

332.6-370.6 K: $\Delta Hf° = -139.196 + 13.889\times10^{-3}T - 2.786\times10^{-6}T^2 + 614.400T^{-1}$
$\Delta Gf° = -139.196 - 13.889\times10^{-3}T\ln T + 2.786\times10^{-6}T^2 + 307.200T^{-1} + 146.483\times10^{-3}T$

370.6-529 K: $\Delta Hf° = -134.159 + 11.883\times10^{-3}T - 1.810\times10^{-6}T^2 - 29.700T^{-1}$
$\Delta Gf° = -134.159 - 11.883\times10^{-3}T\ln T + 1.810\times10^{-6}T^2 - 14.850T^{-1} + 123.732\times10^{-3}T$

Sources: Enthalpy of formation from Gross (93). Enthalpy of sublimation at 298 K from JANAF (63). Other data from Webb (258).

$AlBr_3(g)$

Aluminum Tribromide (ideal gas)

[Formation: $Al(c,l) + 1.5Br_2(l,g) = AlBr_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	18.015	83.492	83.492	0	-98.100	-104.703	76.749
300	18.033	83.604	83.494	.033	-98.128	-104.744	76.305
332.6	18.261	85.476	83.598	.625	-98.610	-105.439	69.282
332.6	18.261	85.476	83.598	.625	-109.207	-105.439	69.282
400	18.732	88.898	84.211	1.875	-109.246	-104.675	57.191
500	19.107	93.123	85.585	3.769	-109.299	-103.527	45.251
600	19.326	96.627	87.140	5.692	-109.359	-102.364	37.286
700	19.464	99.618	88.715	7.632	-109.441	-101.193	31.593
800	19.557	102.223	90.244	9.583	-109.551	-100.007	27.320
900	19.621	104.530	91.706	11.542	-109.701	-98.807	23.993
933.61	19.636	105.250	92.180	12.202	-109.760	-98.399	23.034
933.61	19.636	105.250	92.180	12.202	-112.340	-98.399	23.034
1000	19.667	106.600	93.093	13.507	-112.436	-97.404	21.287
1100	19.702	108.476	94.408	15.475	-112.580	-95.894	19.052
1200	19.729	110.192	95.653	17.447	-112.722	-94.370	17.187
1300	19.750	111.772	96.833	19.421	-112.864	-92.836	15.607
1400	19.766	113.236	97.952	21.397	-113.006	-91.288	14.250
1500	19.780	114.600	99.017	23.374	-113.150	-89.734	13.074
1600	19.791	115.877	100.031	25.353	-113.294	-88.166	12.043
1700	19.800	117.077	100.999	27.332	-113.438	-86.594	11.132
1800	19.808	118.209	101.924	29.313	-113.583	-85.009	10.321
1900	19.814	119.281	102.810	31.294	-113.729	-83.415	9.595
2000	19.820	120.297	103.660	33.275	-113.878	-81.819	8.941

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.675 + 0.116\times10^{-3}T - 1.506\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.675\times10^{-3}T + 0.058\times10^{-6}T^2 + 1.506\times10^{2}T^{-1} - 6.376$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -94.935 - 12.053\times10^{-3}T - 1.519\times10^{-6}T^2 + 168.000T^{-1}$

$\Delta Gf^\circ = -94.935 + 12.053\times10^{-3}T\ln T + 1.519\times10^{-6}T^2 + 84.000T^{-1} - 102.838\times10^{-3}T$

332.6-933.61 K: $\Delta Hf^\circ = -109.935 + 1.688\times10^{-3}T - 1.752\times10^{-6}T^2 + 120.900T^{-1}$

$\Delta Gf^\circ = -109.935 - 1.688\times10^{-3}T\ln T + 1.752\times10^{-6}T^2 + 60.450T^{-1} + 22.195\times10^{-3}T$

933.61-2000 K: $\Delta Hf^\circ = -111.203 - 1.310\times10^{-3}T - 0.024\times10^{-6}T^2 + 103.500T^{-1}$

$\Delta Gf^\circ = -111.203 + 1.310\times10^{-3}T\ln T + 0.024\times10^{-6}T^2 + 51.750T^{-1} + 4.672\times10^{-3}T$

Source: Data from JANAF (63).

$(AlBr_3)_2(g)$

Dimeric Aluminum Tribromide (ideal gas)

[Formation: $2Al(c,l) + 3Br_2(l,g) = (AlBr_3)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	40.037	130.763	130.763	0	-224.000	-226.407	165.959
300	40.075	131.010	130.763	.074	-224.047	-226.421	164.945
332.6	40.544	135.168	130.995	1.388	-224.880	-226.637	148.920
332.6	40.544	135.168	130.995	1.388	-246.075	-226.637	148.920
400	41.513	142.761	132.356	4.162	-245.881	-222.725	121.690
500	42.255	152.112	135.404	8.354	-245.583	-216.971	94.837
600	42.682	159.857	138.852	12.603	-245.300	-211.271	76.954
700	42.947	166.458	142.337	16.885	-245.061	-205.620	64.197
800	43.123	172.205	145.719	21.189	-244.880	-199.998	54.636
900	43.246	177.292	148.950	25.508	-244.778	-194.398	47.206
933.61	43.276	178.878	149.999	26.962	-244.761	-192.517	45.066
933.61	43.276	178.878	149.999	26.962	-249.921	-192.517	45.066
1000	43.334	181.853	152.016	29.837	-249.849	-188.438	41.183
1100	43.400	185.986	154.919	34.174	-249.736	-182.302	36.220
1200	43.450	189.765	157.667	38.517	-249.620	-176.174	32.085
1300	43.489	193.244	160.272	42.864	-249.506	-170.060	28.589
1400	43.520	196.468	162.744	47.214	-249.392	-163.950	25.593
1500	43.546	199.472	165.093	51.568	-249.280	-157.855	22.999
1600	43.567	202.283	167.331	55.923	-249.170	-151.762	20.729
1700	43.584	204.925	169.466	60.281	-249.060	-145.681	18.728
1800	43.598	207.416	171.505	64.640	-248.952	-139.600	16.950
1900	43.610	209.774	173.458	69.000	-248.846	-133.522	15.358
2000	43.621	212.011	175.330	73.362	-248.744	-127.460	13.928

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 43.426 + 0.172\times10^{-3}T - 3.058\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 43.426\times10^{-3}T + 0.086\times10^{-6}T^2 + 3.058\times10^{2}T^{-1} - 13.981$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -218.897 - 20.031\times10^{-3}T - 3.068\times10^{-6}T^2 + 340.600T^{-1}$

$\Delta Gf^\circ = -218.897 + 20.031\times10^{-3}T\ln T + 3.068\times10^{-6}T^2 + 170.300T^{-1} - 142.147\times10^{-3}T$

332.6-933.61 K: $\Delta Hf^\circ = -248.899 + 7.452\times10^{-3}T - 3.533\times10^{-6}T^2 + 246.400T^{-1}$

$\Delta Gf^\circ = -248.899 - 7.452\times10^{-3}T\ln T + 3.533\times10^{-6}T^2 + 123.200T^{-1} + 107.918\times10^{-3}T$

933.61-2000 K: $\Delta Hf^\circ = -251.434 + 1.456\times10^{-3}T - 0.079\times10^{-6}T^2 + 211.600T^{-1}$

$\Delta Gf^\circ = -251.434 - 1.456\times10^{-3}T\ln T + 0.079\times10^{-6}T^2 + 105.800T^{-1} + 72.871\times10^{-3}T$

Source: Data from JANAF (63).

AlCl(g)
Aluminum Monochloride (ideal gas)
[Formation: $Al(c,l) + 0.5Cl_2(g) = AlCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.284	54.457	54.457	0	-12.300	-18.572	13.613
300	8.291	54.508	54.458	.015	-12.304	-18.611	13.558
400	8.560	56.934	54.786	.859	-12.472	-20.689	11.304
500	8.711	58.862	55.416	1.723	-12.659	-22.722	9.932
600	8.804	60.459	56.127	2.599	-12.869	-24.714	9.002
700	8.867	61.821	56.845	3.483	-13.106	-26.669	8.326
800	8.913	63.008	57.543	4.372	-13.378	-28.590	7.810
900	8.948	64.060	58.210	5.265	-13.691	-30.473	7.400
933.61	8.958	64.388	58.427	5.566	-13.805	-31.098	7.280
933.61	8.958	64.388	58.427	5.566	-16.385	-31.097	7.280
1000	8.977	65.004	58.842	6.162	-16.590	-32.136	7.023
1100	9.001	65.861	59.442	7.061	-16.899	-33.677	6.691
1200	9.022	66.645	60.010	7.962	-17.207	-35.188	6.408
1300	9.041	67.368	60.549	8.865	-17.514	-36.675	6.165
1400	9.059	68.039	61.060	9.770	-17.820	-38.137	5.953
1500	9.075	68.664	61.546	10.677	-18.125	-39.577	5.766
1600	9.090	69.250	62.009	11.585	-18.430	-40.997	5.600
1700	9.105	69.802	62.452	12.495	-18.734	-42.398	5.451
1800	9.119	70.323	62.875	13.406	-19.037	-43.782	5.316
1900	9.133	70.816	63.280	14.318	-19.340	-45.147	5.193
2000	9.146	71.285	63.669	15.232	-19.642	-46.499	5.081

Phase change: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.866 + 0.156\times10^{-3}T - 0.559\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.866\times10^{-3}T + 0.078\times10^{-6}T^2 + 0.559\times10^{2}T^{-1} - 2.838$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf^\circ = -12.239 - 0.140\times10^{-3}T - 1.693\times10^{-6}T^2 + 39.150T^{-1}$

$\Delta Gf^\circ = -12.239 + 0.140\times10^{-3}T\ln T + 1.693\times10^{-6}T^2 + 19.575T^{-1} - 22.760\times10^{-3}T$

933.61-2000 K: $\Delta Hf^\circ = -13.507 - 3.138\times10^{-3}T + 0.034\times10^{-6}T^2 + 21.750T^{-1}$

$\Delta Gf^\circ = -13.507 + 3.138\times10^{-3}T\ln T - 0.034\times10^{-6}T^2 + 10.875T^{-1} - 40.283\times10^{-3}T$

Source: Data from JANAF (63).

$AlCl_2(g)$

Aluminum Dichloride (ideal gas)

[Formation: $Al(c,l) + Cl_2(g) = AlCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	12.341	69.146	69.146	0	-67.000	-69.707	51.096
300	12.356	69.222	69.146	.023	-67.003	-69.724	50.793
400	12.932	72.864	69.639	1.290	-67.164	-70.608	38.578
500	13.249	75.787	70.585	2.601	-67.330	-71.448	31.229
600	13.436	78.221	71.661	3.936	-67.515	-72.254	26.318
700	13.555	80.302	72.751	5.286	-67.725	-73.027	22.800
800	13.635	82.117	73.809	6.646	-67.970	-73.769	20.153
900	13.691	83.727	74.825	8.012	-68.254	-74.478	18.086
933.61	13.704	84.229	75.154	8.472	-68.359	-74.708	17.488
933.61	13.704	84.229	75.154	8.472	-70.939	-74.708	17.488
1000	13.731	85.171	75.788	9.383	-71.127	-74.971	16.385
1100	13.762	86.482	76.702	10.758	-71.408	-75.343	14.969
1200	13.785	87.680	77.567	12.135	-71.690	-75.687	13.784
1300	13.803	88.784	78.388	13.515	-71.971	-76.009	12.778
1400	13.818	89.808	79.168	14.896	-72.253	-76.309	11.912
1500	13.830	90.762	79.910	16.278	-72.536	-76.591	11.159
1600	13.839	91.654	80.615	17.662	-72.819	-76.849	10.497
1700	13.847	92.494	81.290	19.046	-73.103	-77.093	9.911
1800	13.854	93.285	81.934	20.431	-73.388	-77.319	9.388
1900	13.860	94.034	82.551	21.817	-73.673	-77.526	8.917
2000	13.865	94.746	83.145	23.203	-73.961	-77.725	8.493

*Data except enthalpy of formation at 298 K estimated.

Phase change: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.692 + 0.136\times10^{-3}T - 1.237\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.692\times10^{-3}T + 0.068\times10^{-6}T^2 + 1.237\times10^{2}T^{-1} - 4.503$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf^\circ = -67.170 + 0.273\times10^{-3}T - 1.747\times10^{-6}T^2 + 72.800T^{-1}$

$\Delta Gf^\circ = -67.170 - 0.273\times10^{-3}T\ln T + 1.747\times10^{-6}T^2 + 36.400T^{-1} - 7.884\times10^{-3}T$

933.61-2000 K: $\Delta Hf^\circ = -68.438 - 2.725\times10^{-3}T - 0.020\times10^{-6}T^2 + 55.400T^{-1}$

$\Delta Gf^\circ = -68.438 + 2.725\times10^{-3}T\ln T + 0.020\times10^{-6}T^2 + 27.700T^{-1} - 25.407\times10^{-3}T$

Source: Data from Chase (26) who estimated molecular constants.

$AlCl_3(c,l)$
Aluminum Trichloride
[Formation: $Al(c) + 1.5Cl_2(g) = AlCl_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	21.780	26.120	26.120	0	-168.650	-150.585	110.380
300	21.820	26.255	26.122	.040	-168.643	-150.473	109.618
400	23.920	32.820	27.003	2.327	-168.199	-144.480	78.939
465.7	29.300	36.560	28.091	3.944	-167.827	-140.611	65.987
465.7	30.000	54.704	28.090	12.394	-159.377	-140.611	65.987
500	30.000	56.836	29.990	13.423	-159.007	-139.242	60.862

Phase changes: 453.8 K, vapor pressure (monomer and dimer) = 1 atm.
465.7 K, melting point of $AlCl_3$; ΔH° = 8.450 kcal/mol.
467 K, triple point; vapor pressure = 2.3 atm.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-465.7 K: $Cp^\circ = 15.520 + 21.000\times10^{-3}T$

$H^\circ - H^\circ_{298} = 15.520\times10^{-3}T + 10.500\times10^{-6}T^2 - 5.561$

465.7-500 K: $Cp^\circ = 30.000$

$H^\circ - H^\circ_{298} = 30.000\times10^{-3}T - 1.577$

Formation equations (kcal/mol):

298.15-465.7 K: $\Delta Hf^\circ = -168.443 - 2.312\times10^{-3}T + 8.641\times10^{-6}T^2 - 85.050T^{-1}$

$\Delta Gf^\circ = -168.443 + 2.312\times10^{-3}T\ln T - 8.641\times10^{-6}T^2 - 42.525T^{-1} + 49.777\times10^{-3}T$

465.7-500 K: $\Delta Hf^\circ = -164.460 + 12.168\times10^{-3}T - 1.859\times10^{-6}T^2 - 85.050T^{-1}$

$\Delta Gf^\circ = -164.460 - 12.168\times10^{-3}T\ln T + 1.859\times10^{-6}T^2 - 42.525T^{-1} + 125.291\times10^{-3}T$

Source: Data from JANAF (63).

$AlCl_3(g)$

Aluminum Trichloride (ideal gas)

[Formation: $Al(c,l) + 1.5Cl_2(g) = AlCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	17.179	75.140	75.140	0	-139.720	-136.270	99.887
300	17.203	75.246	75.140	.032	-139.721	-136.249	99.256
400	18.168	80.341	75.829	1.805	-139.792	-135.081	73.804
500	18.710	84.459	77.155	3.652	-139.848	-133.895	58.525
600	19.035	87.901	78.668	5.540	-139.915	-132.697	48.334
700	19.243	90.852	80.202	7.455	-139.999	-131.488	41.052
800	19.383	93.432	81.700	9.386	-140.115	-130.267	35.587
900	19.482	95.721	83.132	11.330	-140.266	-129.027	31.332
933.61	19.506	96.436	83.598	11.985	-140.326	-128.606	30.105
933.61	19.506	96.436	83.598	11.985	-142.906	-128.606	30.105
1000	19.554	97.777	84.495	13.282	-143.006	-127.587	27.884
1100	19.608	99.643	85.788	15.240	-143.152	-126.038	25.041
1200	19.649	101.351	87.015	17.203	-143.298	-124.475	22.670
1300	19.681	102.925	88.179	19.170	-143.443	-122.900	20.661
1400	19.707	104.385	89.286	21.139	-143.589	-121.315	18.938
1500	19.728	105.745	90.338	23.111	-143.735	-119.719	17.443
1600	19.745	107.019	91.341	25.085	-143.882	-118.113	16.133
1700	19.760	108.217	92.299	27.060	-144.030	-116.497	14.977
1800	19.772	109.346	93.215	29.036	-144.179	-114.874	13.947
1900	19.782	110.416	94.093	31.014	-144.328	-113.239	13.025
2000	19.790	111.431	94.935	32.993	-144.480	-111.600	12.195

Phase change: 933.61 K, melting point of Al; $\Delta H^\circ = 2.580$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.473 + 0.240\times10^{-3}T - 2.106\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.473\times10^{-3}T + 0.120\times10^{-6}T^2 + 2.106\times10^{2}T^{-1} - 6.523$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf^\circ = -140.476 + 1.641\times10^{-3}T - 1.739\times10^{-6}T^2 + 125.550T^{-1}$

$\Delta Gf^\circ = -140.476 - 1.641\times10^{-3}T\ln T + 1.739\times10^{-6}T^2 + 62.775T^{-1} + 22.228\times10^{-3}T$

933.61-2000 K: $\Delta Hf^\circ = -141.743 - 1.357\times10^{-3}T - 0.012\times10^{-6}T^2 + 108.150T^{-1}$

$\Delta Gf^\circ = -141.743 + 1.357\times10^{-3}T\ln T + 0.012\times10^{-6}T^2 + 54.075T^{-1} + 4.704\times10^{-3}T$

Source: Data from JANAF (63).

$(AlCl_3)_2(g)$

Dimeric Aluminum Trichloride (ideal gas)

[Formation: $2Al(c,l) + 3Cl_2(g) = (AlCl_3)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	37.968	113.514	113.514	0	-309.690	-291.828	213.913
300	38.023	113.749	113.516	.070	-309.687	-291.718	212.514
400	40.172	125.015	115.035	3.992	-309.451	-285.763	156.132
500	41.330	134.116	117.972	8.072	-309.178	-279.871	122.330
600	42.011	141.717	121.314	12.242	-308.917	-274.032	99.815
700	42.442	148.227	124.704	16.466	-308.691	-268.236	83.746
800	42.729	153.915	128.007	20.726	-308.527	-262.472	71.703
900	42.930	158.960	131.172	25.009	-308.434	-256.721	62.340
933.61	42.979	160.535	132.201	26.453	-308.420	-254.790	59.643
933.61	42.979	160.535	132.201	26.453	-313.580	-254.790	59.643
1000	43.076	163.491	134.181	29.310	-313.515	-250.614	54.771
1100	43.185	167.602	137.036	33.623	-313.411	-244.330	48.543
1200	43.269	171.363	139.741	37.946	-313.306	-238.053	43.355
1300	43.335	174.829	142.308	42.277	-313.199	-231.786	38.966
1400	43.387	178.043	144.748	46.613	-313.093	-225.527	35.206
1500	43.429	181.038	147.069	50.954	-312.988	-219.278	31.948
1600	43.464	183.842	149.281	55.298	-312.886	-213.035	29.099
1700	43.492	186.477	151.391	59.646	-312.783	-206.791	26.585
1800	43.517	188.964	153.410	63.997	-312.683	-200.563	24.351
1900	43.537	191.317	155.344	68.349	-312.585	-194.329	22.353
2000	43.555	193.551	157.199	72.704	-312.493	-188.111	20.556

Phase change: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 43.068 + 0.380\times10^{-3}T - 4.635\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 43.068\times10^{-3}T + 0.190\times10^{-6}T^2 + 4.635\times10^{2}T^{-1} - 14.412$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf^\circ = -312.568 + 7.403\times10^{-3}T - 3.528\times10^{-6}T^2 + 293.400T^{-1}$

$\Delta Gf^\circ = -312.568 - 7.403\times10^{-3}T\ln T + 3.528\times10^{-6}T^2 + 146.700T^{-1} + 109.037\times10^{-3}T$

933.61-2000 K: $\Delta Hf^\circ = -315.103 + 1.407\times10^{-3}T - 0.074\times10^{-6}T^2 + 258.600T^{-1}$

$\Delta Gf^\circ = -315.103 - 1.407\times10^{-3}T\ln T + 0.074\times10^{-6}T^2 + 129.300T^{-1} + 73.990\times10^{-3}T$

Source: Data from JANAF (63).

AlF(g)

Aluminum Monofluoride (ideal gas)

[Formation: $Al(c,l) + 0.5F_2(g) = AlF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	7.632	51.398	51.398	0	-63.500	-69.582	51.005
300	7.640	51.445	51.398	.014	-63.504	-69.621	50.718
400	8.031	53.699	51.701	.799	-63.701	-71.629	39.136
500	8.302	55.522	52.290	1.616	-63.910	-73.587	32.165
600	8.485	57.053	52.960	2.456	-64.136	-75.501	27.501
700	8.613	58.371	53.641	3.311	-64.387	-77.375	24.157
800	8.705	59.528	54.306	4.178	-64.671	-79.212	21.639
900	8.774	60.557	54.944	5.052	-64.992	-81.011	19.672
933.61	8.792	60.879	55.152	5.347	-65.109	-81.607	19.103
933.61	8.792	60.879	55.152	5.347	-67.689	-81.607	19.103
1000	8.828	61.485	55.553	5.932	-67.902	-82.590	18.050
1100	8.871	62.328	56.131	6.817	-68.219	-84.044	16.698
1200	8.907	63.102	56.680	7.706	-68.535	-85.468	15.566
1300	8.937	63.816	57.202	8.598	-68.849	-86.867	14.603
1400	8.962	64.479	57.698	9.493	-69.163	-88.241	13.775
1500	8.985	65.098	58.171	10.391	-69.476	-89.593	13.053
1600	9.006	65.679	58.623	11.290	-69.788	-90.924	12.420
1700	9.024	66.225	59.053	12.192	-70.100	-92.234	11.857
1800	9.041	66.742	59.467	13.095	-70.411	-93.529	11.356
1900	9.057	67.231	59.863	14.000	-70.722	-94.803	10.905
2000	9.072	67.696	60.243	14.906	-71.034	-96.063	10.497

Phase change: 933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 15.460 + 0.396\times10^{-3}T - 0.841\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.460\times10^{-3}T + 0.198\times10^{-6}T^2 + 0.841\times10^{2}T^{-1} - 2.822$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf^\circ = -63.413 - 0.386\times10^{-3}T - 1.616\times10^{-6}T2 + 51.250T^{-1}$

$\Delta Gf^\circ = -63.413 + 0.386\times10^{-3}T\ln T + 1.616\times10^{-6}T^2 + 25.625T^{-1} - 23.661\times10^{-3}T$

933.61-2000 K: $\Delta Hf^\circ = -64.681 - 3.384\times10^{-3}T + 0.111\times10^{-6}T^2 + 33.850T^{-1}$

$\Delta Gf^\circ = -64.681 + 3.384\times10^{-3}T\ln T - 0.111\times10^{-6}T^2 + 16.925T^{-1} - 41.184\times10^{-3}T$

Source: Data from JANAF (63).

$AlF_2(g)$
Aluminum Difluoride (ideal gas)
[Formation: $Al(c,l) + F_2(g) = AlF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	10.960	63.120	63.120	0	-166.000	-168.356	123.406
300	10.979	63.188	63.121	.020	-166.005	-168.371	122.657
400	11.844	66.473	63.563	1.164	-166.228	-169.125	92.405
500	12.420	69.183	64.425	2.379	-166.441	-169.825	74.229
600	12.801	71.483	65.413	3.642	-166.659	-170.480	62.096
700	13.058	73.477	66.426	4.936	-166.895	-171.098	53.418
800	13.239	75.233	67.419	6.251	-167.161	-171.682	46.901
900	13.369	76.800	68.376	7.582	-167.461	-172.228	41.822
933.61	13.401	77.291	68.688	8.032	-167.571	-172.404	40.358
933.61	13.401	77.291	68.688	8.032	-170.151	-172.404	40.358
1000	13.465	78.214	69.290	8.924	-170.349	-172.559	37.712
1100	13.538	79.501	70.161	10.274	-170.644	-172.766	34.325
1200	13.595	80.681	70.989	11.631	-170.937	-172.945	31.497
1300	13.640	81.771	71.777	12.992	-171.230	-173.101	29.100
1400	13.676	82.784	72.528	14.358	-171.523	-173.235	27.043
1500	13.705	83.728	73.243	15.727	-171.816	-173.347	25.256
1600	13.729	84.613	73.926	17.099	-172.109	-173.439	23.690
1700	13.750	85.446	74.580	18.473	-172.402	-173.512	22.306
1800	13.767	86.233	75.206	19.849	-172.697	-173.570	21.074
1900	13.781	86.978	75.806	21.226	-172.992	-173.609	19.969
2000	13.794	87.685	76.382	22.605	-173.289	-173.635	18.974

*Data except enthalpy of formation at 298 K estimated.

Phase change: 933.61 K, melting point of Al; $\Delta H^\circ = 2.580$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 12.985 + 0.566\times10^{-3}T - 1.950\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 12.985\times10^{-3}T + 0.283\times10^{-6}T^2 + 1.950\times10^{2}T^{-1} - 4.551$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf^\circ = -166.197 - 0.115\times10^{-3}T - 1.618\times10^{-6}T^2 + 111.900T^{-1}$

$\Delta Gf^\circ = -166.197 + 0.115\times10^{-3}T\ln T + 1.618\times10^{-6}T^2 + 55.950T^{-1} - 9.007\times10^{-3}T$

933.61-2000 K: $\Delta Hf^\circ = -167.465 - 3.113\times10^{-3}T + 0.109\times10^{-6}T^2 + 94.500T^{-1}$

$\Delta Gf^\circ = -167.465 + 3.113\times10^{-3}T\ln T - 0.109\times10^{-6}T^2 + 47.250T^{-1} - 26.530\times10^{-3}T$

Source: Data from Chase (26) who estimated molecular constants.

$AlF_3(c)$
Aluminum Trifluoride
[Formation: $Al(c,l) + 1.5F_2(g) = AlF_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	17.950	15.890	15.890	0	-361.000	-342.052	250.728
300	18.013	16.001	15.891	.033	-360.999	-341.936	249.097
400	20.619	21.577	16.632	1.978	-360.806	-335.604	183.363
500	22.058	26.347	18.111	4.118	-360.495	-329.338	143.952
600	23.247	30.470	19.835	6.381	-360.128	-323.140	117.702
700	25.211	34.184	21.623	8.793	-359.671	-317.009	98.973
728	26.044	35.189	22.126	9.510	-359.511	-315.306	94.655
728	23.321	35.374	22.126	9.645	-359.376	-315.306	94.655
800	23.541	37.584	23.420	11.331	-359.145	-310.961	84.950
900	23.833	40.373	25.151	13.700	-358.842	-304.955	74.052
933.61	23.925	41.249	25.715	14.503	-358.747	-302.944	70.916
933.61	23.925	41.249	25.715	14.503	-361.327	-302.944	70.916
1000	24.107	42.899	26.802	16.097	-361.115	-298.803	65.302
1100	24.365	45.209	28.373	18.520	-360.780	-292.588	58.131
1200	24.605	47.339	29.865	20.969	-360.427	-286.403	52.160
1300	24.829	49.318	31.286	23.441	-360.056	-280.249	47.114
1400	25.036	51.165	32.641	25.934	-359.672	-274.125	42.792
1500	25.226	52.899	33.934	28.447	-359.273	-268.030	39.051
1600	25.398	54.533	35.171	30.979	-358.858	-261.959	35.782

Phase changes: 728 K, α - β transition point of AlF_3; $\Delta H° = 0.135$ kcal/mol.
933.61 K, melting point of Al; $\Delta H° = 2.580$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-728 K: $Cp° = 19.228 + 8.746\times10^{-3}T - 3.454\times10^{5}T^{-2}$

$H°- H°_{298} = 19.228\times10^{-3}T + 4.373\times10^{-6}T^2 + 3.454\times10^{2}T^{-1} - 7.280$

728-1600 K: $Cp° = 22.500 + 1.912\times10^{-3}T - 3.024\times10^{5}T^{-2}$

$H°- H°_{298} = 22.500\times10^{-3}T + 0.956\times10^{-6}T^2 + 3.024\times10^{2}T^{-1} - 7.657$

Formation equations (kcal/mol):

298.15-728 K: $\Delta Hf° = -362.482 + 1.874\times10^{-3}T + 2.385\times10^{-6}T^2 + 212.050T^{-1}$

$\Delta Gf° = -362.482 - 1.874\times10^{-3}T\ln T - 2.385\times10^{-6}T^2 + 106.025T^{-1} + 78.717\times10^{-3}T$

728-933.61 K: $\Delta Hf° = -362.859 + 5.146\times10^{-3}T - 1.032\times10^{-6}T^2 + 169.050T^{-1}$

$\Delta Gf° = -362.859 - 5.146\times10^{-3}T\ln T + 1.032\times10^{-6}T^2 + 84.525T^{-1} + 98.351\times10^{-3}T$

933.61-1600 K: $\Delta Hf° = -364.127 + 2.148\times10^{-3}T + 0.695\times10^{-6}T^2 + 151.650T^{-1}$

$\Delta Gf° = -364.127 - 2.148\times10^{-3}T\ln T - 0.695\times10^{-6}T^2 + 75.825T^{-1} + 80.828\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from CODATA (34). Low-temperature heat capacities and entropy at 298 K from King (126). High-temperature data based on Douglas (58).

$AlF_3(g)$

Aluminum Trifluoride (ideal gas)

[Formation: $Al(c,l) + 1.5F_2(g) = AlF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	14.945	66.150	66.150	0	-289.400	-285.437	209.229
300	14.977	66.243	66.150	.028	-289.404	-285.413	207.921
400	16.402	70.760	66.757	1.601	-289.582	-284.054	155.198
500	17.352	74.530	67.946	3.292	-289.721	-282.656	123.547
600	17.985	77.753	69.318	5.061	-289.848	-281.230	102.437
700	18.418	80.560	70.727	6.883	-289.980	-279.782	87.351
800	18.723	83.040	72.114	8.741	-290.134	-278.316	76.031
900	18.943	85.259	73.455	10.624	-290.318	-276.828	67.222
933.61	18.998	85.955	73.892	11.262	-290.388	-276.323	64.684
933.61	18.998	85.955	73.892	11.262	-292.968	-276.323	64.684
1000	19.107	87.264	74.737	12.527	-293.085	-275.137	60.130
1100	19.232	89.091	75.959	14.445	-293.255	-273.333	54.306
1200	19.329	90.769	77.125	16.373	-293.423	-271.515	49.449
1300	19.406	92.319	78.234	18.310	-293.587	-269.681	45.337
1400	19.468	93.760	79.293	20.254	-293.752	-267.838	41.811
1500	19.518	95.104	80.302	22.203	-293.917	-265.981	38.753
1600	19.560	96.365	81.267	24.157	-294.080	-264.112	36.076
1700	19.594	97.552	82.190	26.115	-294.243	-262.233	33.712
1800	19.624	98.673	83.075	28.076	-294.410	-260.346	31.610
1900	19.649	99.735	83.925	30.039	-294.575	-258.448	29.728
2000	19.670	100.743	84.740	32.005	-294.743	-256.543	28.033

Phase change: 933.61 K, melting point of Al; $\Delta H° = 2.580$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 18.070 + 1.168\times10^{-3}T - 3.088\times10^{5}T^{-2}$

$H°- H°_{298} = 18.070\times10^{-3}T + 0.584\times10^{-6}T^2 + 3.088\times10^{2}T^{-1} - 6.475$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = -290.077 + 0.716\times10^{-3}T - 1.404\times10^{-6}T^2 + 175.450T^{-1}$

$\Delta Gf° = -290.077 - 0.716\times10^{-3}T\ln T + 1.404\times10^{-6}T^2 + 87.725T^{-1} + 18.236\times10^{-3}T$

933.61-2000 K: $\Delta Hf° = -291.345 - 2.282\times10^{-3}T + 0.323\times10^{-6}T^2 + 158.050T^{-1}$

$\Delta Gf° = -291.345 + 2.282\times10^{-3}T\ln T - 0.323\times10^{-6}T^2 + 79.025T^{-1} + 0.712\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (188). Other data from JANAF (60).

$(AlF_3)_2(g)$

Dimeric Aluminum Trifluoride (ideal gas)

[Formation: $2Al(c,l) + 3F_2(g) = (AlF_3)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	31.964	92.476	92.476	0	-628.000	-608.201	445.818
300	32.048	92.674	92.477	.059	-628.005	-608.080	442.980
400	35.684	102.431	93.781	3.460	-628.107	-601.415	328.594
500	37.980	110.660	96.356	7.152	-628.075	-594.744	259.959
600	39.466	117.725	99.343	11.029	-627.990	-588.084	214.207
700	40.462	123.889	102.419	15.029	-627.898	-581.440	181.531
800	41.155	129.340	105.451	19.111	-627.840	-574.811	157.029
900	41.653	134.217	108.380	23.253	-627.831	-568.181	137.971
933.61	41.777	135.746	109.338	24.655	-627.843	-565.952	132.483
933.61	41.777	135.746	109.338	24.655	-633.003	-565.952	132.483
1000	42.022	138.626	111.188	27.438	-632.986	-561.189	122.646
1100	42.301	142.645	113.868	31.655	-632.945	-554.010	110.070
1200	42.518	146.335	116.422	35.896	-632.895	-546.836	99.591
1300	42.689	149.745	118.855	40.157	-632.837	-539.665	90.725
1400	42.826	152.914	121.177	44.432	-632.780	-532.504	83.126
1500	42.938	155.873	123.392	48.721	-632.718	-525.345	76.542
1600	43.030	158.647	125.510	53.019	-632.656	-518.187	70.780
1700	43.107	161.258	127.537	57.326	-632.591	-511.033	65.697
1800	43.171	163.723	129.479	61.640	-632.531	-503.883	61.179
1900	43.226	166.059	131.343	65.960	-632.468	-496.734	57.137
2000	43.273	168.278	133.135	70.285	-632.412	-489.596	53.500

Phase change: 933.61 K, melting point of Al; $\Delta H° = 2.580$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 40.138 + 2.260\times10^{-3}T - 7.865\times10^{5}T^{-2}$

$H°- H°_{298} = 40.138\times10^{-3}T + 1.130\times10^{-6}T^2 + 7.865\times10^{2}T^{-1} - 14.706$

Formation equations (kcal/mol):

298.15-933.61 K: $\Delta Hf° = -631.109 + 5.430\times10^{-3}T - 2.846\times10^{-6}T^2 + 519.800T^{-1}$

$\Delta Gf° = -631.109 - 5.430\times10^{-3}T\ln T + 2.846\times10^{-6}T^2 + 259.900T^{-1} + 104.000\times10^{-3}T$

933.61-2000 K: $\Delta Hf° = -633.645 - 0.566\times10^{-3}T + 0.608\times10^{-6}T^2 + 485.000T^{-1}$

$\Delta Gf° = -633.645 + 0.566\times10^{-3}T\ln T - 0.608\times10^{-6}T^2 + 242.500T^{-1} + 68.953\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Other data from JANAF (60).

AlI(g)
Aluminum Monoiodide (ideal gas)
[Formation: $Al(c,l) + 0.5I_2(c,l,g) = AlI(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.635	59.207	59.207	0	16.240	4.746	-3.479
300	8.639	59.260	59.207	.016	16.233	4.674	-3.405
386.8	8.770	61.474	59.478	.772	15.868	1.376	-.777
386.8	8.770	61.474	59.478	.772	14.013	1.376	-.777
400	8.790	61.769	59.549	.888	13.921	.946	-.517
458.4	8.838	62.971	59.909	1.404	13.513	-.918	.438
458.4	8.838	62.971	59.909	1.404	8.503	-.918	.438
500	8.872	63.740	60.196	1.772	8.422	-1.769	.773
600	8.923	65.362	60.925	2.662	8.213	-3.787	1.379
700	8.959	66.740	61.660	3.556	7.975	-5.768	1.801
800	8.987	67.938	62.372	4.453	7.703	-7.713	2.107
900	9.010	68.998	63.050	5.353	7.391	-9.623	2.337
933.61	9.017	69.328	63.270	5.656	7.276	-10.256	2.401
933.61	9.017	69.328	63.270	5.656	4.696	-10.256	2.401
1000	9.030	69.949	63.694	6.255	4.490	-11.312	2.472
1100	9.048	70.810	64.302	7.159	4.181	-12.878	2.559
1200	9.064	71.598	64.878	8.064	3.873	-14.415	2.625
1300	9.080	72.324	65.422	8.972	3.567	-15.926	2.677
1400	9.095	72.998	65.941	9.880	3.260	-17.415	2.719
1500	9.109	73.626	66.432	10.791	2.956	-18.882	2.751
1600	9.123	74.214	66.900	11.702	2.651	-20.327	2.776
1700	9.137	74.768	67.347	12.615	2.347	-21.755	2.797
1800	9.150	75.290	67.773	13.530	2.045	-23.162	2.812
1900	9.164	75.785	68.182	14.445	1.741	-24.553	2.824
2000	9.177	76.256	68.575	15.362	1.439	-25.931	2.834

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
933.61 K, melting point of Al; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.925 + 0.132\times10^{-3}T - 0.293\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.925\times10^{-3}T + 0.066\times10^{-6}T^2 + 0.293\times10^{2}T^{-1} - 2.765$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = 16.925 - 2.105\times10^{-3}T - 2.407\times10^{-6}T^2 + 46.700T^{-1}$

$\Delta Gf^\circ = 16.925 + 2.105\times10^{-3}T\ln T + 2.407\times10^{-6}T^2 + 23.350T^{-1} - 53.826\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = 16.198 - 5.308\times10^{-3}T - 1.661\times10^{-6}T^2 + 46.700T^{-1}$

$\Delta Gf^\circ = 16.198 + 5.308\times10^{-3}T\ln T + 1.661\times10^{-6}T^2 + 23.350T^{-1} - 70.734\times10^{-3}T$

458.4-933.61 K: $\Delta Hf^\circ = 8.841 - 0.138\times10^{-3}T - 1.695\times10^{-6}T^2 + 39.050T^{-1}$

$\Delta Gf^\circ = 8.841 + 0.138\times10^{-3}T\ln T + 1.695\times10^{-6}T^2 + 19.525T^{-1} - 23.003\times10^{-3}T$

933.61-2000 K: $\Delta Hf^\circ = 7.573 - 3.136\times10^{-3}T + 0.032\times10^{-6}T^2 + 21.650T^{-1}$

$\Delta Gf^\circ = 7.573 + 3.136\times10^{-3}T\ln T - 0.032\times10^{-6}T^2 + 10.825T^{-1} - 40.526\times10^{-3}T$

Source: Data from JANAF (63).

AlI_3(c,l)

Aluminum Triiodide

[Formation: $Al(c) + 1.5I_2(c,l,g) = AlI_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	23.700	38.000	38.000	0	-72.400	-69.295	50.794
300	23.700	38.146	38.000	.044	-72.403	-69.276	50.467
386.8	25.436	44.380	38.753	2.177	-72.600	-68.348	38.617
386.8	25.436	44.380	38.753	2.177	-78.163	-68.348	38.617
400	25.700	45.238	38.953	2.514	-78.289	-68.011	37.159
458.4	26.886	48.819	39.986	4.049	-78.802	-66.470	31.690
458.4	26.886	48.819	39.986	4.049	-93.834	-66.470	31.690
464	27.000	49.146	40.094	4.200	-93.793	-66.136	31.151
464	30.000	57.767	40.094	8.200	-89.793	-66.136	31.151
500	30.000	60.009	41.449	9.280	-89.424	-64.313	28.111
600	30.000	65.478	45.011	12.280	-88.421	-59.385	21.631

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
464 K, melting point of AlI_3; $\Delta H°$ = 4.000 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-464 K: $Cp° = 17.678 + 20.058\times10^{-3}T$

$H°- H°_{298} = 17.678\times10^{-3}T + 10.029\times10^{-6}T^2 - 6.162$

464-600 K: $Cp° = 30.000$

$H°- H°_{298} = 30.000\times10^{-3}T - 5.720$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -71.140 - 6.229\times10^{-3}T + 6.064\times10^{-6}T^2 + 17.400T^{-1}$

$\Delta Gf° = -71.140 + 6.229\times10^{-3}T\ln T - 6.064\times10^{-6}T^2 + 8.700T^{-1} - 27.596\times10^{-3}T$

386.8-458.4 K: $\Delta Hf° = -73.323 - 15.836\times10^{-3}T + 8.302\times10^{-6}T^2 + 17.400T^{-1}$

$\Delta Gf° = -73.323 + 15.836\times10^{-3}T\ln T - 8.302\times10^{-6}T^2 + 8.700T^{-1} - 78.319\times10^{-3}T$

458.4-464 K: $\Delta Hf° = -95.393 - 0.325\times10^{-3}T + 8.200\times10^{-6}T^2 - 5.550T^{-1}$

$\Delta Gf° = -95.393 + 0.325\times10^{-3}T\ln T - 8.200\times10^{-6}T^2 - 2.775T^{-1} + 64.876\times10^{-3}T$

464-600 K: $\Delta Hf° = -94.951 + 11.997\times10^{-3}T - 1.829\times10^{-6}T2 - 5.550T^{-1}$

$\Delta Gf° = -94.951 - 11.997\times10^{-3}T\ln T + 1.829\times10^{-6}T^2 - 2.775T^{-1} + 134.926\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Efimov (72). Entropy at 298 K from Wagman (252). Other data based on Fischer (80).

$AlI_3(g)$
Aluminum Triiodide (ideal gas)
[Formation: $Al(c,l) + 1.5I_2(c,l,g) = AlI_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	18.423	89.270	89.270	0	-46.200	-58.382	42.794
300	18.437	89.384	89.271	.034	-46.213	-58.457	42.585
386.8	18.923	94.138	89.849	1.659	-46.918	-61.912	34.981
386.8	18.923	94.138	89.849	1.659	-52.481	-61.912	34.981
400	18.997	94.774	90.002	1.909	-52.694	-62.230	34.001
458.4	19.168	97.378	90.778	3.025	-53.626	-63.554	30.300
458.4	19.168	97.378	90.778	3.025	-68.658	-63.554	30.300
500	19.289	99.048	91.398	3.825	-68.679	-63.087	27.575
600	19.458	102.581	92.976	5.763	-68.738	-61.964	22.570
700	19.564	105.589	94.569	7.714	-68.817	-60.829	18.991
800	19.634	108.206	96.114	9.674	-68.928	-59.680	16.304
900	19.683	110.522	97.589	11.640	-69.078	-58.517	14.210
933.61	19.695	111.244	98.067	12.302	-69.137	-58.122	13.606
933.61	19.695	111.244	98.067	12.302	-71.717	-58.122	13.606
1000	19.718	112.598	98.987	13.611	-71.814	-57.150	12.490
1100	19.744	114.478	100.311	15.584	-71.961	-55.678	11.062
1200	19.764	116.197	101.564	17.559	-72.108	-54.191	9.869
1300	19.780	117.780	102.752	19.537	-72.253	-52.691	8.858
1400	19.793	119.246	103.878	21.515	-72.402	-51.180	7.990
1500	19.803	120.612	104.949	23.495	-72.550	-49.662	7.236
1600	19.811	121.890	105.967	25.476	-72.699	-48.128	6.574
1700	19.818	123.092	106.941	27.457	-72.851	-46.590	5.990
1800	19.824	124.225	107.870	29.439	-73.004	-45.041	5.469
1900	19.829	125.296	108.758	31.422	-73.158	-43.480	5.001
2000	19.833	126.314	109.612	33.405	-73.314	-41.916	4.580

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
933.61 K, melting point of Al; $\Delta H°$ = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.747 + 0.074\times10^{-3}T - 1.196\times10^{5}T^{-2}$

$H°- H°_{298} = 19.747\times10^{-3}T + 0.037\times10^{-6}T^{2} + 1.196\times10^{2}T^{-1} - 6.292$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -45.070 - 4.160\times10^{-3}T - 3.928\times10^{-6}T^{2} + 137.000T^{-1}$

$\Delta Gf° = -45.070 + 4.160\times10^{-3}T\ln T + 3.928\times10^{-6}T^{2} + 68.500T^{-1} - 70.294\times10^{-3}T$

386.8-458.4 K: $\Delta Hf° = -47.253 - 13.767\times10^{-3}T - 1.690\times10^{-6}T^{2} + 137.000T^{-1}$

$\Delta Gf° = -47.253 + 13.767\times10^{-3}T\ln T + 1.690\times10^{-6}T^{2} + 68.500T^{-1} - 121.017\times10^{-3}T$

458.4-933.61 K: $\Delta Hf° = -69.322 + 1.744\times10^{-3}T - 1.792\times10^{-6}T^{2} + 114.050T^{-1}$

$\Delta Gf° = -69.322 - 1.744\times10^{-3}T\ln T + 1.792\times10^{-6}T^{2} + 57.025T^{-1} + 22.177\times10^{-3}T$

933.61-2000 K: $\Delta Hf° = -70.590 - 1.254\times10^{-3}T - 0.065\times10^{-6}T^{2} + 96.650T^{-1}$

$\Delta Gf° = -70.590 + 1.254\times10^{-3}T\ln T + 0.065\times10^{-6}T^{2} + 48.325T^{-1} + 4.654\times10^{-3}T$

Source: Data from JANAF (63).

$(AlI_3)_2(g)$

Dimeric Aluminum Triiodide (ideal gas)

[Formation: $2Al(c,l) + 3I_2(c,l,g) = (AlI_3)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	41.098	142.751	142.751	0	-117.000	-130.693	95.799
300	41.126	143.006	142.753	.076	-117.018	-130.778	95.270
386.8	42.039	153.587	144.042	3.692	-118.061	-134.632	76.069
386.8	42.039	153.587	144.042	3.692	-129.188	-134.632	76.069
400	42.178	155.000	144.380	4.248	-129.558	-134.812	73.657
458.4	42.487	160.774	146.108	6.723	-131.180	-135.458	64.581
458.4	42.487	160.774	146.108	6.723	-161.243	-135.458	64.581
500	42.707	164.474	147.484	8.495	-161.113	-133.119	58.185
600	43.006	172.290	150.987	12.782	-160.819	-127.548	46.459
700	43.190	178.934	154.517	17.092	-160.570	-122.023	38.097
800	43.311	184.709	157.937	21.418	-160.385	-116.527	31.833
900	43.396	189.816	161.202	25.753	-160.282	-111.056	26.968
933.61	43.416	191.407	162.260	27.212	-160.265	-109.219	25.567
933.61	43.416	191.407	162.260	27.212	-165.425	-109.219	25.567
1000	43.456	194.391	164.295	30.096	-165.354	-105.222	22.996
1100	43.501	198.535	167.222	34.444	-165.245	-99.216	19.712
1200	43.536	202.322	169.992	38.796	-165.138	-93.217	16.977
1300	43.562	205.808	172.615	43.151	-165.028	-87.228	14.664
1400	43.584	209.037	175.103	47.508	-164.925	-81.246	12.683
1500	43.601	212.045	177.467	51.867	-164.823	-75.279	10.968
1600	43.615	214.859	179.716	56.228	-164.722	-69.306	9.467
1700	43.627	217.504	181.863	60.590	-164.626	-63.348	8.144
1800	43.637	219.997	183.912	64.953	-164.532	-57.392	6.968
1900	43.645	222.357	185.874	69.318	-164.442	-51.440	5.917
2000	43.652	224.596	187.755	73.682	-164.356	-45.496	4.972

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
933.61 K, melting point of Al; $\Delta H°$ = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 43.548 + 0.106\times10^{-3}T - 2.206\times10^{5}T^{-2}$

$H°- H°_{298} = 43.548\times10^{-3}T + 0.053\times10^{-6}T^2 + 2.206\times10^{2}T^{-1} - 13.728$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -115.884 - 4.267\times10^{-3}T - 7.877\times10^{-6}T^2 + 255.400T^{-1}$

$\Delta Gf° = -115.884 + 4.267\times10^{-3}T\ln T + 7.877\times10^{-6}T^2 + 127.700T^{-1} - 77.764\times10^{-3}T$

386.8-458.4 K: $\Delta Hf° = -120.250 - 23.479\times10^{-3}T - 3.401\times10^{-6}T^2 + 255.400T^{-1}$

$\Delta Gf° = -120.250 + 23.479\times10^{-3}T\ln T + 3.401\times10^{-6}T^2 + 127.700T^{-1} - 179.210\times10^{-3}T$

458.4-933.61 K: $\Delta Hf° = -164.389 + 7.541\times10^{-3}T - 3.605\times10^{-6}T^2 + 209.500T^{-1}$

$\Delta Gf° = -164.389 - 7.541\times10^{-3}T\ln T + 3.605\times10^{-6}T^2 + 104.750T^{-1} + 107.179\times10^{-3}T$

933.61-2000 K: $\Delta Hf° = -166.925 + 1.545\times10^{-3}T - 0.151\times10^{-6}T^2 + 174.700T^{-1}$

$\Delta Gf° = -166.925 - 1.545\times10^{-3}T\ln T + 0.151\times10^{-6}T^2 + 87.350T^{-1} + 72.132\times10^{-3}T$

Source: Data from JANAF (63).

$AsBr_3(g)$

Arsenic Tribromide (ideal gas)

[Formation: $As[\alpha, 1/4As_4(g)] + 1.5Br_2(l,g) = AsBr_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	18.880	86.860	86.860	0	-31.000	-38.083	27.915
300	18.900	86.980	86.863	.035	-31.025	-38.128	27.776
332.6	19.030	88.936	86.972	.653	-31.482	-38.876	25.545
332.6	19.030	88.936	86.972	.653	-42.080	-38.876	25.545
400	19.300	92.480	87.610	1.948	-42.076	-38.231	20.888
500	19.500	96.810	89.032	3.889	-42.070	-37.270	16.291
600	19.610	100.370	90.628	5.845	-42.074	-36.306	13.224
700	19.680	103.400	92.243	7.810	-42.088	-35.346	11.035
800	19.720	106.030	93.805	9.780	-42.114	-34.379	9.392
876	19.750	107.826	94.949	11.280	-42.144	-33.650	8.395
876	19.750	107.826	94.949	11.280	-50.453	-33.650	8.395
900	19.760	108.360	95.300	11.754	-50.420	-33.190	8.060
1000	19.780	110.440	96.709	13.731	-50.286	-31.281	6.836

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
876 K, sublimation point of As(c) to $As_4(g)$; ΔH° = 33.235 kcal/mol of $As_4(g)$.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 19.810 + 0.056\times10^{-3}T - 0.842\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.810\times10^{-3}T + 0.028\times10^{-6}T^2 + 0.842\times10^{2}T^{-1} - 6.191$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -27.325 - 13.018\times10^{-3}T - 0.393\times10^{-6}T^2 + 71.800T^{-1}$

$\Delta Gf^\circ = -27.325 + 13.018\times10^{-3}T\ln T + 0.393\times10^{-6}T^2 + 35.900T^{-1} - 110.774\times10^{-3}T$

332.6-876 K: $\Delta Hf^\circ = -42.325 + 0.724\times10^{-3}T - 0.625\times10^{-6}T^2 + 24.700T^{-1}$

$\Delta Gf^\circ = -42.325 - 0.724\times10^{-3}T\ln T + 0.625\times10^{-6}T^2 + 12.350T^{-1} + 14.259\times10^{-3}T$

876-1000 K: $\Delta Hf^\circ = -51.817 + 1.587\times10^{-3}T - 0.102\times10^{-6}T^2 + 46.200T^{-1}$

$\Delta Gf^\circ = -51.817 - 1.587\times10^{-3}T\ln T + 0.102\times10^{-6}T^2 + 23.100T^{-1} + 31.386\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). All other data from Clark (32).

$AsCl_3(g)$

Arsenic Trichloride (ideal gas)

[Formation: $As[_\alpha, 1/4As_4(g)] + 1.5Cl_2(g) = AsCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.020	78.130	78.130	0	-62.500	-59.417	43.554
300	18.040	78.240	78.130	.033	-62.500	-59.398	43.271
400	18.770	83.540	78.845	1.878	-62.501	-58.364	31.888
500	19.140	87.770	80.218	3.776	-62.495	-57.326	25.057
600	19.360	91.280	81.777	5.702	-62.500	-56.292	20.504
700	19.490	94.280	83.359	7.645	-62.514	-55.261	17.253
800	19.580	96.890	84.893	9.598	-62.542	-54.226	14.814
876	19.626	98.669	86.012	11.088	-62.572	-53.435	13.331
876	19.626	98.669	86.012	11.088	-70.881	-53.435	13.331
900	19.640	99.200	86.357	11.559	-70.849	-52.958	12.860
1000	19.680	101.270	87.744	13.526	-70.715	-50.976	11.141

Phase change: 876 K, sublimation point of As(c) to $As_4(g)$; $\Delta H°$ = 33.235 kcal/mol of $As_4(g)$.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 19.623 + 0.226\times10^{-3}T - 1.485\times10^{5}T^{-2}$

$H°- H°_{298} = 19.623\times10^{-3}T + 0.113\times10^{-6}T^2 + 1.485\times10^{2}T^{-1} - 6.359$

Formation equations (kcal/mol):

298.15-876 K: $\Delta Hf° = -62.767 + 0.691\times10^{-3}T - 0.590\times10^{-6}T^2 + 33.650T^{-1}$

$\Delta Gf° = -62.767 - 0.691\times10^{-3}T\ln T + 0.590\times10^{-6}T^2 + 16.825T^{-1} + 14.808\times10^{-3}T$

876-1000 K: $\Delta Hf° = -72.258 + 1.554\times10^{-3}T - 0.066\times10^{-6}T^2 + 55.150T^{-1}$

$\Delta Gf° = -72.258 - 1.554\times10^{-3}T\ln T + 0.066\times10^{-6}T^2 + 27.575T^{-1} + 31.935\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252, 255). All other data from Clark (32).

$AsF_3(g)$
Arsenic Trifluoride (ideal gas)
[Formation: $As[\alpha, 1/4As_4(g)] + 1.5F_2(g) = AsF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	15.460	68.990	68.990	0	-187.800	-184.160	134.991
300	15.490	69.090	68.993	.029	-187.803	-184.139	134.143
400	16.950	73.760	69.618	1.657	-187.929	-182.895	99.928
500	17.830	77.640	70.842	3.399	-188.006	-181.624	79.387
600	18.380	80.950	72.263	5.212	-188.064	-180.346	65.690
700	18.740	83.810	73.711	7.069	-188.120	-179.055	55.903
800	18.990	86.330	75.135	8.956	-188.179	-177.757	48.560
876	19.119	88.063	76.185	10.405	-188.226	-176.767	44.100
876	19.119	88.063	76.185	10.405	-196.535	-176.767	44.100
900	19.160	88.580	76.509	10.864	-196.509	-176.226	42.793
1000	19.290	90.600	77.813	12.787	-196.399	-173.974	38.022

Phase change: 876 K, sublimation point of As(c) to $As_4(g)$; ΔH° = 33.235 kcal/mol of $As_4(g)$.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 18.036 + 1.698\times10^{-3}T - 2.740\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 18.036\times10^{-3}T + 0.849\times10^{-6}T^2 + 2.740\times10^{2}T^{-1} - 6.372$

Formation equations (kcal/mol):

298.15-876 K: $\Delta Hf^\circ = -188.049 - 0.417\times10^{-3}T + 0.017\times10^{-6}T^2 + 110.850T^{-1}$

$\Delta Gf^\circ = -188.049 + 0.417\times10^{-3}T\ln T - 0.017\times10^{-6}T^2 + 55.425T^{-1} + 10.049\times10^{-3}T$

876-1000 K: $\Delta Hf^\circ = -197.541 + 0.446\times10^{-3}T + 0.541\times10^{-6}T^2 + 132.350T^{-1}$

$\Delta Gf^\circ = -197.541 - 0.446\times10^{-3}T\ln T - 0.541\times10^{-6}T^2 + 66.175T^{-1} + 27.177\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252, 255). All other data from Clark (32).

AsI_3(c,l)

Arsenic Triiodide

[Formation: $As(\alpha) + 1.5I_2(c,l,g) = AsI_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	25.280	50.920	50.920	0	-13.900	-14.123	10.353
300	25.308	51.076	50.920	.047	-13.900	-14.124	10.289
386.8	26.629	57.669	51.720	2.301	-13.978	-14.183	8.013
386.8	26.629	57.669	51.720	2.301	-19.541	-14.183	8.013
400	26.830	58.566	51.931	2.654	-19.651	-13.998	7.648
413.6	27.037	59.466	52.164	3.020	-19.761	-13.804	7.294
413.6	32.900	72.329	52.164	8.340	-14.441	-13.804	7.294
458.4	32.900	75.712	54.302	9.814	-14.534	-13.726	6.544
458.4	32.900	75.712	54.302	9.814	-29.566	-13.726	6.544
500	32.900	78.570	56.204	11.183	-29.012	-12.310	5.381
600	32.900	84.569	60.447	14.473	-27.694	-9.096	3.313
700*	32.900	89.640	64.264	17.763	-26.393	-6.099	1.904

*AsI_3 vaporizes with decomposition, Rusin (202).

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
413.6 K, melting point of AsI_3; ΔH° = 5.320 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-413.6 K: $Cp^\circ = 20.744 + 15.218\times10^{-3}T$

$H^\circ - H^\circ_{298} = 20.744\times10^{-3}T + 7.609\times10^{-6}T^2 - 6.861$

413.6-700 K: $Cp^\circ = 32.900$

$H^\circ - H^\circ_{298} = 32.900\times10^{-3}T - 5.267$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -13.014 - 4.262\times10^{-3}T + 4.800\times10^{-6}T^2 - 12.400T^{-1}$

$\Delta Gf^\circ = -13.014 + 4.262\times10^{-3}T\ln T - 4.800\times10^{-6}T^2 - 6.200T^{-1} - 26.505\times10^{-3}T$

386.8-413.6 K: $\Delta Hf^\circ = -15.197 - 13.869\times10^{-3}T + 7.038\times10^{-6}T^2 - 12.400T^{-1}$

$\Delta Gf^\circ = -15.197 + 13.869\times10^{-3}T\ln T - 7.038\times10^{-6}T^2 - 6.200T^{-1} - 77.228\times10^{-3}T$

413.6-458.4 K: $\Delta Hf^\circ = -13.603 - 1.713\times10^{-3}T - 0.571\times10^{-6}T^2 - 12.400T^{-1}$

$\Delta Gf^\circ = -13.603 + 1.713\times10^{-3}T\ln T + 0.571\times10^{-6}T^2 - 6.200T^{-1} - 10.990\times10^{-3}T$

458.4-700 K: $\Delta Hf^\circ = -35.673 + 13.798\times10^{-3}T - 0.673\times10^{-6}T^2 - 35.350T^{-1}$

$\Delta Gf^\circ = -35.673 - 13.798\times10^{-3}T\ln T + 0.673\times10^{-6}T^2 - 17.675T^{-1} + 132.204\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (252). Other data from Cubicciotti (47).

$AsI_3(g)$

Arsenic Triiodide (ideal gas)

[Formation: $As[\alpha, 1/4As_4(g)] + 1.5I_2(c,1,g) = AsI_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	19.350	93.620	93.620	0	9.300	-3.654	2.679
300	19.350	93.740	93.620	.036	9.289	-3.734	2.721
386.8	19.541	98.694	94.232	1.726	8.647	-7.426	4.196
386.8	19.541	98.694	94.232	1.726	3.083	-7.426	4.196
400	19.570	99.350	94.390	1.984	2.879	-7.782	4.252
458.4	19.634	102.022	95.196	3.129	1.981	-9.272	4.420
458.4	19.634	102.022	95.196	3.129	-13.051	-9.272	4.420
500	19.680	103.730	95.836	3.947	-13.048	-8.926	3.902
600	19.740	107.320	97.457	5.918	-13.049	-8.102	2.951
700	19.770	110.370	99.093	7.894	-13.062	-7.279	2.273
800	19.800	113.010	100.670	9.872	-13.088	-6.449	1.762
876	19.808	114.805	101.816	11.378	-13.118	-5.817	1.451
876	19.808	114.805	101.816	11.378	-21.427	-5.817	1.451
900	19.810	115.340	102.170	11.853	-21.396	-5.389	1.309
1000	19.820	117.430	103.595	13.835	-21.264	-3.619	.791

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
876 K, sublimation point of As(c) to $As_4(g)$; ΔH° = 33.235 kcal/mol of $As_4(g)$.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 19.834 + 0.040\times10^{-3}T - 0.441\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.834\times10^{-3}T + 0.020\times10^{-6}T^2 + 0.441\times10^{2}T^{-1} - 6.063$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = 10.984 - 5.173\times10^{-3}T - 2.789\times10^{-6}T^2 + 31.700T^{-1}$

$\Delta Gf^\circ = 10.984 + 5.173\times10^{-3}T\ln T + 2.789\times10^{-6}T^2 + 15.850T^{-1} - 79.577\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = 8.801 - 14.779\times10^{-3}T - 0.551\times10^{-6}T^2 + 31.700T^{-1}$

$\Delta Gf^\circ = 8.801 + 14.779\times10^{-3}T\ln T + 0.551\times10^{-6}T^2 + 15.850T^{-1} - 130.300\times10^{-3}T$

458.4-876 K: $\Delta Hf^\circ = -13.269 + 0.731\times10^{-3}T - 0.653\times10^{-6}T^2 + 8.750T^{-1}$

$\Delta Gf^\circ = -13.269 - 0.731\times10^{-3}T\ln T + 0.653\times10^{-6}T^2 + 4.375T^{-1} + 12.894\times10^{-3}T$

876-1000 K: $\Delta Hf^\circ = -22.760 + 1.594\times10^{-3}T - 0.129\times10^{-6}T^2 + 30.250T^{-1}$

$\Delta Gf^\circ = -22.760 - 1.594\times10^{-3}T\ln T + 0.129\times10^{-6}T^2 + 15.125T^{-1} + 30.022\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Alikhanyan (2) and Cubicciotti (47). All other data from Clark (32).

BBr(g)
Boron Monobromide (ideal gas)
[Formation: $B(\beta) + 0.5Br_2(l,g) = BBr(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	7.837	53.750	53.750	0	56.900	46.718	-34.245
300	7.845	53.799	53.750	.015	56.894	46.656	-33.989
332.6	7.966	54.615	53.795	.273	56.765	45.551	-29.931
332.6	7.966	54.615	53.795	.273	53.233	45.551	-29.931
400	8.216	56.111	54.063	.819	53.260	43.987	-24.033
500	8.451	57.971	54.665	1.653	53.246	41.671	-18.214
600	8.604	59.526	55.349	2.506	53.180	39.359	-14.336
700	8.708	60.861	56.044	3.372	53.081	37.064	-11.572
800	8.783	62.029	56.720	4.247	52.963	34.786	-9.503
900	8.839	63.067	57.369	5.128	52.825	32.521	-7.897
1000	8.883	64.000	57.985	6.015	52.674	30.275	-6.617
1100	8.918	64.849	58.572	6.905	52.509	28.036	-5.570
1200	8.947	65.626	59.128	7.798	52.331	25.821	-4.703
1300	8.972	66.343	59.655	8.694	52.141	23.623	-3.971
1400	8.994	67.009	60.158	9.592	51.938	21.436	-3.346
1500	9.014	67.630	60.635	10.493	51.722	19.270	-2.808
1600	9.032	68.212	61.090	11.395	51.492	17.102	-2.336
1700	9.048	68.761	61.526	12.299	51.249	14.959	-1.923
1800	9.064	69.278	61.942	13.205	50.993	12.845	-1.560
1900	9.078	69.769	62.342	14.112	50.724	10.734	-1.235
2000	9.092	70.235	62.725	15.020	50.441	8.622	-.942

Phase change: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.654 + 0.274\times10^{-3}T - 0.799\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.654\times10^{-3}T + 0.137\times10^{-6}T^2 + 0.799\times10^{2}T^{-1} - 2.860$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = 58.872 - 4.968\times10^{-3}T - 0.567\times10^{-6}T^2 - 131.400T^{-1}$

$\Delta Gf^\circ = 58.872 + 4.968\times10^{-3}T\ln T + 0.567\times10^{-6}T^2 - 65.700T^{-1} - 68.505\times10^{-3}T$

332.6-2000 K: $\Delta Hf^\circ = 53.872 - 0.388\times10^{-3}T - 0.645\times10^{-6}T^2 - 147.100T^{-1}$

$\Delta Gf^\circ = 53.872 + 0.388\times10^{-3}T\ln T + 0.645\times10^{-6}T^2 - 73.550T^{-1} - 26.827\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Other data from JANAF (60).

$BBr_2(g)$
Boron Dibromide (ideal gas)
[Formation: $B(\beta) + Br_2(l,g) = BBr_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	11.486	70.402	70.402	0	15.000	5.276	-3.868
300	11.503	70.473	70.403	.021	14.983	5.217	-3.801
332.6	11.746	71.672	70.470	.400	14.682	4.171	-2.741
332.6	11.746	71.672	70.470	.400	7.617	4.171	-2.741
400	12.248	73.892	70.865	1.211	7.614	3.468	-1.895
500	12.726	76.680	71.756	2.462	7.576	2.438	-1.066
600	13.035	79.030	72.778	3.751	7.502	1.414	-.515
700	13.242	81.056	73.819	5.066	7.406	.409	-.128
800	13.385	82.834	74.838	6.397	7.296	-.582	.159
900	13.488	84.416	75.815	7.741	7.172	-1.560	.379
1000	13.564	85.842	76.748	9.094	7.037	-2.523	.551
1100	13.621	87.137	77.633	10.454	6.891	-3.477	.691
1200	13.666	88.325	78.477	11.818	6.733	-4.411	.803
1300	13.701	89.420	79.277	13.186	6.562	-5.330	.896
1400	13.729	90.436	80.037	14.558	6.380	-6.237	.974
1500	13.752	91.384	80.763	15.932	6.183	-7.128	1.039
1600	13.771	92.272	81.455	17.308	5.972	-8.020	1.095
1700	13.786	93.108	82.116	18.686	5.748	-8.889	1.143
1800	13.799	93.896	82.749	20.065	5.510	-9.731	1.181
1900	13.811	94.642	83.355	21.446	5.259	-10.566	1.215
2000	13.820	95.351	83.938	22.827	4.992	-11.408	1.247

*Enthalpy of formation at 298 K estimated.

Phase change: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.230 + 0.420\times10^{-3}T - 1.661\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.230\times10^{-3}T + 0.210\times10^{-6}T^2 + 1.661\times10^{2}T^{-1} - 4.520$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = 18.005 - 9.438\times10^{-3}T - 0.444\times10^{-6}T^2 - 45.200T^{-1}$

$\Delta Gf^\circ = 18.005 + 9.438\times10^{-3}T\ln T + 0.444\times10^{-6}T^2 - 22.600T^{-1} - 96.344\times10^{-3}T$

332.6-2000 K: $\Delta Hf^\circ = 8.005 - 0.277\times10^{-3}T - 0.599\times10^{-6}T^2 - 76.600T^{-1}$

$\Delta Gf^\circ = 8.005 + 0.277\times10^{-3}T\ln T + 0.599\times10^{-6}T^2 - 38.300T^{-1} - 12.989\times10^{-3}T$

Source: Data from JANAF (60) who estimated enthalpy of formation at 298 K and some molecular constants.

$BBr_3(g)$

Boron Tribromide (ideal gas)

[Formation: $B(\beta) + 1.5Br_2(l,g) = BBr_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	16.198	77.487	77.487	0	-48.800	-55.213	40.472
300	16.224	77.588	77.488	.030	-48.825	-55.251	40.250
332.6	16.594	79.281	77.582	.565	-49.264	-55.927	36.749
332.6	16.594	79.281	77.582	.565	-59.861	-55.927	36.749
400	17.358	82.423	78.140	1.713	-59.821	-55.140	30.127
500	18.079	86.380	79.404	3.488	-59.777	-53.973	23.591
600	18.545	89.720	80.852	5.321	-59.750	-52.817	19.238
700	18.857	92.604	82.330	7.192	-59.737	-51.662	16.129
800	19.074	95.137	83.776	9.089	-59.729	-50.507	13.798
900	19.230	97.393	85.165	11.005	-59.730	-49.355	11.985
1000	19.345	99.425	86.491	12.934	-59.739	-48.201	10.534
1100	19.432	101.273	87.752	14.873	-59.757	-47.052	9.348
1200	19.499	102.967	88.951	16.819	-59.785	-45.894	8.358
1300	19.553	104.530	90.090	18.772	-59.823	-44.733	7.520
1400	19.595	105.980	91.173	20.730	-59.872	-43.568	6.801
1500	19.630	107.334	92.207	22.691	-59.936	-42.399	6.178
1600	19.659	108.602	93.192	24.656	-60.013	-41.239	5.633
1700	19.683	109.794	94.133	26.623	-60.103	-40.063	5.150
1800	19.703	110.920	95.036	28.592	-60.206	-38.870	4.719
1900	19.720	111.985	95.899	30.563	-60.323	-37.676	4.334
2000	19.735	112.997	96.729	32.536	-60.455	-36.496	3.988

Phase changes: 227.2 K, melting point of BBr_3; ΔH° unknown.
332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
364.4 K, boiling point of BBr_3; ΔH° = 7.30 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 18.723 + 0.750\times10^{-3}T - 2.444\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 18.723\times10^{-3}T + 0.375\times10^{-6}T^2 + 2.444\times10^{2}T^{-1} - 6.435$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -45.018 - 12.991\times10^{-3}T - 0.229\times10^{-6}T^2 + 33.100T^{-1}$

$\Delta Gf^\circ = -45.018 + 12.991\times10^{-3}T\ln T + 0.229\times10^{-6}T^2 + 16.550T^{-1} - 108.464\times10^{-3}T$

332.6-2000 K: $\Delta Hf^\circ = -60.018 + 0.751\times10^{-3}T - 0.461\times10^{-6}T^2 - 14.000T^{-1}$

$\Delta Gf^\circ = -60.018 - 0.751\times10^{-3}T\ln T + 0.461\times10^{-6}T^2 - 7.000T^{-1} + 16.569\times10^{-3}T$

Source: Data from JANAF (60).

BCl(g)
Boron Monochloride (ideal gas)
[Formation: $B(\beta) + 0.5Cl_2(g) = BCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	7.567	50.942	50.942	0	35.730	28.906	-21.189
300.00	7.575	50.988	50.942	.014	35.731	28.865	-21.028
400.00	7.967	53.224	51.244	.792	35.778	26.565	-14.514
500.00	8.248	55.034	51.826	1.604	35.756	24.266	-10.607
600.00	8.442	56.556	52.491	2.439	35.681	21.972	-8.003
700.00	8.579	57.868	53.168	3.290	35.576	19.696	-6.149
800.00	8.678	59.020	53.829	4.153	35.450	17.437	-4.763
900.00	8.752	60.047	54.464	5.025	35.308	15.194	-3.690
1000.00	8.810	60.972	55.069	5.903	35.151	12.968	-2.834
1100.00	8.856	61.814	55.645	6.786	34.981	10.751	-2.136
1200.00	8.894	62.586	56.191	7.674	34.800	8.558	-1.559
1300.00	8.926	63.300	56.712	8.565	34.606	6.382	-1.073
1400.00	8.954	63.962	57.206	9.459	34.400	4.219	-.659
1500.00	8.978	64.581	57.677	10.356	34.181	2.074	-.302
1600.00	9.000	65.161	58.127	11.255	33.948	-.070	.010
1700.00	9.020	65.707	58.556	12.156	33.703	-2.187	.281
1800.00	9.038	66.223	58.968	13.059	33.444	-4.279	.520
1900.00	9.054	66.712	59.363	13.963	33.172	-6.366	.732
2000.00	9.070	67.177	59.743	14.869	32.887	-8.454	.924

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.433 + 0.406\times10^{-3}T - 0.878\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.433\times10^{-3}T + 0.203\times10^{-6}T^2 + 0.878\times10^{2}T^{-1} - 2.827$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = 36.478 - 0.558\times10^{-3}T - 0.595\times10^{-6}T^2 - 157.650T^{-1}$

$\Delta Gf^\circ = 36.478 + 0.558\times10^{-3}T\ln T + 0.595\times10^{-6}T^2 - 78.825T^{-1} - 27.862\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Other data from JANAF (60).

$BCl_2(g)$
Boron Dichloride (ideal gas)
[Formation: $B(\beta) + Cl_2(g) = BCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	11.323	65.144	65.144	0	-19.000	-22.114	16.210
300	11.342	65.214	65.144	.021	-18.999	-22.132	16.123
400	12.170	68.599	65.599	1.200	-18.967	-23.185	12.667
500	12.684	71.375	66.487	2.444	-18.983	-24.236	10.593
600	13.011	73.718	67.501	3.730	-19.041	-25.284	9.210
700	13.227	75.741	68.537	5.043	-19.124	-26.316	8.216
800	13.375	77.518	69.550	6.374	-19.225	-27.337	7.468
900	13.481	79.099	70.525	7.717	-19.341	-28.343	6.882
1000	13.558	80.524	71.455	9.069	-19.471	-29.337	6.412
1100	13.617	81.819	72.339	10.428	-19.613	-30.323	6.024
1200	13.663	83.006	73.179	11.792	-19.768	-31.288	5.698
1300	13.699	84.101	73.978	13.160	-19.936	-32.238	5.420
1400	13.729	85.117	74.738	14.531	-20.117	-33.178	5.179
1500	13.755	86.066	75.462	15.906	-20.311	-34.101	4.968
1600	13.778	86.954	76.153	17.282	-20.521	-35.025	4.784
1700	13.800	87.790	76.813	18.661	-20.743	-35.922	4.618
1800	13.821	88.579	77.445	20.042	-20.979	-36.797	4.468
1900	13.842	89.327	78.050	21.426	-21.227	-37.666	4.333
2000	13.864	90.038	78.632	22.811	-21.491	-38.539	4.211

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.263 + 0.404\times10^{-3}T - 1.831\times10^{5}T^{-2}$

$H°- H°_{298} = 13.263\times10^{-3}T + 0.202\times10^{-6}T^{2} + 1.831\times10^{2}T^{-1} - 4.586$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -18.577 - 0.141\times10^{-3}T - 0.640\times10^{-6}T^{2} - 96.500T^{-1}$

$\Delta Gf° = -18.577 + 0.141\times10^{-3}T\ln T + 0.640\times10^{-6}T^{2} - 48.250T^{-1} - 12.313\times10^{-3}T$

Source: Data from Chase (25) who estimated some molecular constants.

$(BCl_2)_2(g)$
Dimeric Boron Dichloride (ideal gas)
[Formation: $2B(\beta) + 2Cl_2(g) = (BCl_2)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	22.667	85.767	85.767	0	-117.200	-110.154	80.744
300	22.719	85.907	85.767	.042	-117.198	-110.108	80.213
400	25.048	92.780	86.688	2.437	-117.097	-107.765	58.879
500	26.603	98.546	88.498	5.024	-117.030	-105.434	46.085
600	27.649	103.493	90.595	7.739	-117.003	-103.123	37.562
700	28.332	107.808	92.752	10.539	-116.995	-100.808	31.473
800	28.870	111.628	94.878	13.400	-116.998	-98.496	26.907
900	29.217	115.049	96.932	16.305	-117.011	-96.181	23.356
1000	29.511	118.143	98.901	19.242	-117.038	-93.865	20.514
1100	29.684	120.964	100.780	22.202	-117.080	-91.558	18.191
1200	29.840	123.554	102.572	25.178	-117.142	-89.232	16.251
1300	29.978	125.948	104.280	28.169	-117.223	-86.897	14.608
1400	30.099	128.174	105.908	31.173	-117.323	-84.560	13.200
1500	30.203	130.254	107.462	34.188	-117.446	-82.208	11.978
1600	30.263	132.205	108.948	37.212	-117.594	-79.877	10.911
1700	30.319	134.041	110.370	40.241	-117.767	-77.509	9.964
1800	30.370	135.775	111.733	43.275	-117.967	-75.114	9.120
1900	30.417	137.418	113.042	46.315	-118.191	-72.720	8.365
2000	30.460	138.979	114.300	49.359	-118.445	-70.347	7.687

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 28.034 + 1.670\times10^{-3}T - 5.213\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 28.034\times10^{-3}T + 0.835\times10^{-6}T^2 + 5.213\times10^{2}T^{-1} - 10.181$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -117.363 + 1.226\times10^{-3}T - 0.849\times10^{-6}T^2 - 37.900T^{-1}$

$\Delta Gf^\circ = -117.363 - 1.226\times10^{-3}T\ln T + 0.849\times10^{-6}T^2 - 18.950T^{-1} + 31.125\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Other data from JANAF (60).

$BCl_3(g)$

Boron Trichloride (ideal gas)

[Formation: $B(\beta) + 1.5Cl_2(g) = BCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	14.912	69.328	69.328	0	-96.500	-92.917	68.109
300	14.944	69.420	69.328	.028	-96.499	-92.893	67.672
400	16.353	73.926	69.934	1.597	-96.493	-91.696	50.100
500	17.298	77.683	71.117	3.283	-96.493	-90.493	39.554
600	17.935	80.897	72.485	5.047	-96.507	-89.294	32.525
700	18.373	83.697	73.893	6.863	-96.527	-88.090	27.503
800	18.684	86.172	75.276	8.717	-96.548	-86.883	23.735
900	18.910	88.386	76.612	10.597	-96.572	-85.673	20.804
1000	19.079	90.388	77.891	12.497	-96.601	-84.462	18.459
1100	19.208	92.212	79.110	14.412	-96.635	-83.251	16.540
1200	19.308	93.888	80.273	16.338	-96.678	-82.031	14.940
1300	19.388	95.437	81.381	18.273	-96.730	-80.805	13.584
1400	19.452	96.876	82.437	20.215	-96.792	-79.578	12.422
1500	19.504	98.220	83.445	22.163	-96.866	-78.342	11.414
1600	19.547	99.480	84.408	24.115	-96.954	-77.116	10.533
1700	19.583	100.666	85.330	26.072	-97.053	-75.870	9.754
1800	19.614	101.787	86.214	28.032	-97.165	-74.612	9.059
1900	19.640	102.848	87.061	29.995	-97.290	-73.351	8.437
2000	19.662	103.856	87.876	31.960	-97.432	-72.102	7.879

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 18.166 + 1.038\times10^{-3}T - 3.167\times10^{5}T^{-2}$

$H°- H°_{298} = 18.166\times10^{-3}T + 0.519\times10^{-6}T^{2} + 3.167\times10^{2}T^{-1} - 6.525$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -96.581 + 0.349\times10^{-3}T - 0.367\times10^{-6}T^{2} + 2.950T^{-1}$

$\Delta Gf° = -96.581 - 0.349\times10^{-3}T\ln T + 0.367\times10^{-6}T^{2} + 1.475T^{-1} + 14.149\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Other data from JANAF (60).

BF(g)
Boron Monofluoride (ideal gas)
[Formation: $B(\beta) + 0.5F_2(g) = BF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	7.073	47.890	47.890	0	-29.200	-35.836	26.268
300	7.076	47.934	47.891	.013	-29.199	-35.877	26.136
400	7.309	50.000	48.170	.732	-29.182	-38.110	20.822
500	7.581	51.660	48.708	1.476	-29.247	-40.333	17.629
600	7.832	53.065	49.320	2.247	-29.366	-42.543	15.496
700	8.042	54.288	49.944	3.041	-29.514	-44.726	13.964
800	8.211	55.374	50.556	3.854	-29.678	-46.888	12.809
900	8.348	56.349	51.147	4.682	-29.854	-49.028	11.905
1000	8.457	57.234	51.711	5.523	-30.041	-51.148	11.178
1100	8.546	58.045	52.251	6.373	-30.238	-53.256	10.581
1200	8.620	58.792	52.766	7.231	-30.445	-55.338	10.078
1300	8.681	59.484	53.256	8.097	-30.660	-57.398	9.649
1400	8.732	60.129	53.724	8.967	-30.888	-59.448	9.280
1500	8.776	60.733	54.171	9.843	-31.127	-61.475	8.957
1600	8.814	61.301	54.600	10.722	-31.379	-63.503	8.674
1700	8.848	61.836	55.010	11.605	-31.642	-65.501	8.421
1800	8.877	62.343	55.403	12.492	-31.917	-67.474	8.192
1900	8.903	62.824	55.781	13.381	-32.204	-69.440	7.987
2000	8.927	63.281	56.145	14.272	-32.506	-71.405	7.803

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 7.405 + 0.968\times10^{-3}T - 0.552\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 7.405\times10^{-3}T + 0.484\times10^{-6}T^2 + 0.552\times10^{2}T^{-1} - 2.436$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -28.051 - 1.426\times10^{-3}T - 0.357\times10^{-6}T^2 - 206.350T^{-1}$

$\Delta Gf^\circ = -28.051 + 1.426\times10^{-3}T\ln T + 0.357\times10^{-6}T^2 - 103.175T^{-1} - 33.183\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Other data from JANAF (60).

$BF_2(g)$

Boron Difluoride (ideal gas)

[Formation: $B(\beta) + F_2(g) = BF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	9.693	59.046	59.046	0	-141.000	-143.741	105.364
300	9.710	59.106	59.046	.018	-141.001	-143.757	104.726
400	10.614	62.026	59.438	1.035	-141.070	-144.668	79.042
500	11.351	64.477	60.207	2.135	-141.181	-145.553	63.620
600	11.909	66.598	61.100	3.299	-141.322	-146.418	53.332
700	12.322	68.467	62.021	4.512	-141.475	-147.254	45.974
800	12.628	70.133	62.933	5.760	-141.635	-148.068	40.450
900	12.859	71.634	63.817	7.035	-141.800	-148.861	36.148
1000	13.035	72.999	64.669	8.330	-141.973	-149.637	32.703
1100	13.172	74.248	65.483	9.641	-142.152	-150.400	29.881
1200	13.280	75.399	66.263	10.963	-142.340	-151.141	27.526
1300	13.366	76.465	67.007	12.296	-142.536	-151.861	25.530
1400	13.436	77.458	67.718	13.636	-142.744	-152.572	23.817
1500	13.494	78.387	68.398	14.983	-142.963	-153.262	22.330
1600	13.542	79.260	69.051	16.335	-143.195	-153.953	21.029
1700	13.583	80.082	69.676	17.691	-143.439	-154.617	19.877
1800	13.617	80.859	70.275	19.051	-143.697	-155.255	18.850
1900	13.647	81.596	70.852	20.414	-143.967	-155.888	17.931
2000	13.673	82.297	71.407	21.780	-144.252	-156.522	17.104

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 11.678 + 1.336\times10^{-3}T - 2.119\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 11.678\times10^{-3}T + 0.668\times10^{-6}T^2 + 2.119\times10^{2}T^{-1} - 4.252$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -140.222 - 1.407\times10^{-3}T - 0.260\times10^{-6}T^2 - 99.900T^{-1}$

$\Delta Gf^\circ = -140.222 + 1.407\times10^{-3}T\ln T + 0.260\times10^{-6}T^2 - 49.950T^{-1} - 19.333\times10^{-3}T$

Source: Data from Chase (25).

$(BF_2)_2(g)$
Dimeric Boron Difluoride (ideal gas)
[Formation: $2B(\beta) + 2F_2(g) = (BF_2)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	18.378	76.093	76.093	0	-344.200	-337.160	247.142
300	18.436	76.207	76.094	.034	-344.204	-337.115	245.585
400	21.204	81.907	76.852	2.022	-344.388	-334.727	182.884
500	23.313	86.876	78.370	4.253	-344.579	-332.284	145.239
600	24.896	91.274	80.162	6.667	-344.775	-329.813	120.133
700	26.077	95.205	82.035	9.219	-344.955	-327.302	102.187
800	26.964	98.747	83.906	11.873	-345.117	-324.767	88.721
900	27.638	101.964	85.736	14.605	-345.265	-322.212	78.243
1000	28.157	104.904	87.509	17.395	-345.411	-319.645	69.857
1100	28.563	107.607	89.214	20.232	-345.554	-317.072	62.996
1200	28.886	110.107	90.853	23.105	-345.701	-314.473	57.273
1300	29.145	112.430	92.425	26.007	-345.857	-311.857	52.427
1400	29.357	114.598	93.932	28.933	-346.027	-309.238	48.274
1500	29.531	116.629	95.378	31.877	-346.215	-306.595	44.670
1600	29.676	118.540	96.766	34.838	-346.422	-303.971	41.520
1700	29.798	120.343	98.101	37.812	-346.648	-301.307	38.735
1800	29.902	122.049	99.384	40.797	-346.899	-298.610	36.256
1900	29.990	123.668	100.620	43.792	-347.170	-295.916	34.038
2000	30.066	125.208	101.811	46.795	-347.469	-293.237	32.043

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 24.317 + 3.832\times10^{-3}T - 6.295\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 24.317\times10^{-3}T + 1.916\times10^{-6}T^2 + 6.295\times10^{2}T^{-1} - 9.532$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -343.673 - 1.853\times10^{-3}T + 0.060\times10^{-6}T^2 + 5.900T^{-1}$

$\Delta Gf^\circ = -343.673 + 1.853\times10^{-3}T\ln T - 0.060\times10^{-6}T^2 + 2.950T^{-1} + 11.271\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Other data from JANAF (60).

$BF_3(g)$

Boron Trifluoride (ideal gas)

[Formation: $B(\beta) + 1.5F_2(g) = BF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.057	60.766	60.766	0	-271.500	-267.532	196.104
300	12.092	60.841	60.768	.022	-271.504	-267.507	194.876
400	13.753	64.556	61.261	1.318	-271.678	-266.149	145.415
500	15.044	67.770	62.248	2.761	-271.849	-264.744	115.718
600	16.030	70.605	63.410	4.317	-272.013	-263.311	95.910
700	16.777	73.134	64.621	5.959	-272.160	-261.847	81.751
800	17.344	75.413	65.831	7.666	-272.293	-260.365	71.127
900	17.779	77.483	67.013	9.423	-272.411	-258.866	62.860
1000	18.117	79.374	68.155	11.219	-272.523	-257.355	56.244
1100	18.383	81.114	69.256	13.044	-272.631	-255.838	50.830
1200	18.595	82.723	70.312	14.893	-272.737	-254.306	46.315
1300	18.766	84.218	71.324	16.762	-272.845	-252.760	42.492
1400	18.905	85.614	72.295	18.646	-272.959	-251.213	39.216
1500	19.021	86.922	73.227	20.542	-273.081	-249.651	36.374
1600	19.117	88.153	74.122	22.449	-273.211	-248.097	33.888
1700	19.199	89.315	74.983	24.365	-273.348	-246.522	31.692
1800	19.268	90.414	75.810	26.288	-273.500	-244.928	29.738
1900	19.327	91.457	76.605	28.218	-273.659	-243.333	27.989
2000	19.378	92.450	77.373	30.153	-273.833	-241.747	26.417

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 15.536 + 2.544\times10^{-3}T - 3.767\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 15.536\times10^{-3}T + 1.272\times10^{-6}T^2 + 3.767\times10^{2}T^{-1} - 6.009$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -271.034 - 1.803\times10^{-3}T + 0.257\times10^{-6}T^2 + 14.650T^{-1}$

$\Delta Gf^\circ = -271.034 + 1.803\times10^{-3}T\ln T - 0.257\times10^{-6}T^2 + 7.325T^{-1} + 1.468\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from CODATA (34). Other data from JANAF (60).

BI(g)

Boron Monoiodide (ideal gas)

[Formation: $B(\beta) + 0.5I_2(c,l,g) = BI(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	8.021	55.604	55.604	0	73.000	60.980	-44.699
300	8.029	55.653	55.604	.015	72.998	60.907	-44.370
386.8	8.322	57.733	55.856	.726	72.835	57.425	-32.446
386.8	8.322	57.733	55.856	.726	70.981	57.425	-32.446
400	8.366	58.013	55.923	.836	70.916	56.963	-31.123
458.4	8.484	59.163	56.263	1.329	70.618	54.950	-26.198
458.4	8.484	59.163	56.263	1.329	65.607	54.950	-26.198
500	8.568	59.904	56.536	1.684	65.598	53.984	-23.596
600	8.696	61.478	57.233	2.547	65.537	51.663	-18.818
700	8.782	62.825	57.938	3.421	65.444	49.359	-15.410
800	8.844	64.002	58.623	4.303	65.330	47.071	-12.859
900	8.891	65.047	59.280	5.190	65.196	44.796	-10.878
1000	8.927	65.985	59.904	6.081	65.046	42.539	-9.297
1100	8.958	66.838	60.497	6.975	64.882	40.288	-8.004
1200	8.983	67.618	61.058	7.872	64.706	38.062	-6.932
1300	9.006	68.338	61.591	8.771	64.517	35.853	-6.027
1400	9.026	69.006	62.097	9.673	64.315	33.656	-5.254
1500	9.044	69.630	62.579	10.577	64.099	31.476	-4.586
1600	9.061	70.214	63.038	11.482	63.869	29.298	-4.002
1700	9.076	70.764	63.476	12.389	63.626	27.145	-3.490
1800	9.091	71.283	63.896	13.297	63.369	25.018	-3.038
1900	9.105	71.775	64.298	14.207	63.100	22.896	-2.634
2000	9.119	72.242	64.683	15.118	62.817	20.775	-2.270

*Data estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.760 + 0.216\times10^{-3}T - 0.714\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.760\times10^{-3}T + 0.108\times10^{-6}T^2 + 0.714\times10^{2}T^{-1} - 2.861$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = 74.265 - 2.255\times10^{-3}T - 1.392\times10^{-6}T^2 - 139.900T^{-1}$

$\Delta Gf^\circ = 74.265 + 2.255\times10^{-3}T\ln T + 1.392\times10^{-6}T^2 - 69.950T^{-1} - 57.038\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = 73.538 - 5.457\times10^{-3}T - 0.646\times10^{-6}T^2 - 139.900T^{-1}$

$\Delta Gf^\circ = 73.538 + 5.457\times10^{-3}T\ln T + 0.646\times10^{-6}T^2 - 69.950T^{-1} - 73.946\times10^{-3}T$

458.4-2000 K: $\Delta Hf^\circ = 66.181 - 0.288\times10^{-3}T - 0.680\times10^{-6}T^2 - 147.550T^{-1}$

$\Delta Gf^\circ = 66.181 + 0.288\times10^{-3}T\ln T + 0.680\times10^{-6}T^2 - 73.775T^{-1} - 26.215\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

$BI_2(g)$

Boron Diiodide (ideal gas)

[Formation: $B(\beta) + I_2(c,l,g) = BI_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	11.731	73.964	73.964	0	58.000	44.644	-32.725
300	11.748	74.037	73.964	.022	57.993	44.563	-32.463
386.8	12.355	77.104	74.337	1.070	57.564	40.727	-23.011
386.8	12.355	77.104	74.337	1.070	53.855	40.727	-23.011
400	12.447	77.520	74.435	1.234	53.716	40.281	-22.008
458.4	12.700	79.237	74.940	1.970	53.098	38.367	-18.292
458.4	12.700	79.237	74.940	1.970	43.077	38.367	-18.292
500	12.880	80.348	75.344	2.502	43.059	37.941	-16.584
600	13.155	82.722	76.380	3.805	42.990	36.921	-13.448
700	13.336	84.765	77.436	5.130	42.898	35.918	-11.214
800	13.461	86.554	78.466	6.470	42.791	34.929	-9.542
900	13.549	88.145	79.455	7.821	42.669	33.953	-8.245
1000	13.615	89.576	80.397	9.179	42.534	32.993	-7.211
1100	13.664	90.876	81.291	10.543	42.387	32.039	-6.366
1200	13.702	92.067	82.140	11.912	42.228	31.108	-5.665
1300	13.732	93.165	82.947	13.284	42.057	30.192	-5.076
1400	13.756	94.183	83.713	14.658	41.871	29.286	-4.572
1500	13.776	95.133	84.443	16.035	41.672	28.397	-4.137
1600	13.792	96.022	85.139	17.413	41.458	27.509	-3.758
1700	13.805	96.859	85.804	18.793	41.230	26.644	-3.425
1800	13.816	97.648	86.440	20.174	40.988	25.805	-3.133
1900	13.826	98.396	87.051	21.556	40.731	24.969	-2.872
2000	13.834	99.105	87.636	22.939	40.460	24.134	-2.637

*Data estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.372 + 0.332\times10^{-3}T - 1.547\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.372\times10^{-3}T + 0.166\times10^{-6}T^2 + 1.547\times10^{2}T^{-1} - 4.520$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = 59.592 - 4.082\times10^{-3}T - 2.080\times10^{-6}T^2 - 56.600T^{-1}$

$\Delta Gf^\circ = 59.592 + 4.082\times10^{-3}T\ln T + 2.080\times10^{-6}T^2 - 28.300T^{-1} - 73.694\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = 58.137 - 10.486\times10^{-3}T - 0.588\times10^{-6}T^2 - 56.600T^{-1}$

$\Delta Gf^\circ = 58.137 + 10.486\times10^{-3}T\ln T + 0.588\times10^{-6}T^2 - 28.300T^{-1} - 107.510\times10^{-3}T$

458.4-2000 K: $\Delta Hf^\circ = 43.423 - 0.146\times10^{-3}T - 0.656\times10^{-6}T^2 - 71.900T^{-1}$

$\Delta Gf^\circ = 43.423 + 0.146\times10^{-3}T\ln T + 0.656\times10^{-6}T^2 - 35.950T^{-1} - 12.047\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

$BI_3(g)$
Boron Triiodide (ideal gas)
[Formation: $B(\beta) + 1.5I_2(c,l,g) = BI_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	16.919	83.322	83.322	0	17.000	4.992	-3.659
300	16.942	83.427	83.324	.031	16.990	4.918	-3.583
386.8	17.793	87.848	83.858	1.543	16.421	1.494	-.844
386.8	17.793	87.848	83.858	1.543	10.857	1.494	-.844
400	17.922	88.447	83.999	1.779	10.663	1.177	-.643
458.4	18.265	90.918	84.726	2.838	9.806	-.142	.068
458.4	18.265	90.918	84.726	2.838	-5.226	-.142	.068
500	18.510	92.515	85.309	3.603	-5.197	.320	-.140
600	18.878	95.924	86.801	5.474	-5.146	1.415	-.516
700	19.119	98.854	88.320	7.374	-5.113	2.507	-.783
800	19.283	101.418	89.799	9.295	-5.089	3.597	-.983
900	19.400	103.697	91.220	11.229	-5.081	4.680	-1.136
1000	19.486	105.745	92.571	13.174	-5.081	5.766	-1.260
1100	19.551	107.606	93.855	15.126	-5.094	6.844	-1.360
1200	19.601	109.309	95.073	17.083	-5.119	7.932	-1.445
1300	19.640	110.880	96.229	19.046	-5.153	9.026	-1.517
1400	19.671	112.336	97.328	21.011	-5.204	10.119	-1.580
1500	19.697	113.694	98.374	22.980	-5.268	11.218	-1.634
1600	19.717	114.966	99.372	24.950	-5.347	12.309	-1.681
1700	19.735	116.162	100.325	26.923	-5.440	13.416	-1.725
1800	19.750	117.291	101.237	28.897	-5.548	14.538	-1.765
1900	19.762	118.359	102.110	30.873	-5.670	15.659	-1.801
2000	19.773	119.373	102.948	32.850	-5.807	16.773	-1.833

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.214 + 0.408\times10^{-3}T - 2.148\times10^{5}T^{-2}$
$H°- H°_{298} = 19.214\times10^{-3}T + 0.204\times10^{-6}T^{2} + 2.148\times10^{2}T^{-1} - 6.467$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = 18.631 - 4.678\times10^{-3}T - 2.788\times10^{-6}T^{2} + 3.500T^{-1}$
$\Delta Gf° = 18.631 + 4.678\times10^{-3}T\ln T + 2.788\times10^{-6}T^{2} + 1.750T^{-1} - 73.252\times10^{-3}T$
386.8-458.4 K: $\Delta Hf° = 16.448 - 14.285\times10^{-3}T - 0.550\times10^{-6}T^{2} + 3.500T^{-1}$
$\Delta Gf° = 16.448 + 14.285\times10^{-3}T\ln T + 0.550\times10^{-6}T^{2} + 1.750T^{-1} - 123.975\times10^{-3}T$
458.4-2000 K: $\Delta Hf° = -5.622 + 1.226\times10^{-3}T - 0.652\times10^{-6}T^{2} - 19.450T^{-1}$
$\Delta Gf° = -5.622 - 1.226\times10^{-3}T\ln T + 0.652\times10^{-6}T^{2} - 9.725T^{-1} + 19.219\times10^{-3}T$

Source: Data from JANAF (60).

BaBr(g)

Barium Monobromide (ideal gas)

[Formation: $Ba(c,l) + 0.5Br_2(l,g) = BaBr(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.842	64.599	64.599	0	-26.400	-35.789	26.234
300	8.844	64.654	64.601	.016	-26.412	-35.847	26.114
332.6	8.867	65.568	64.651	.305	-26.643	-36.860	24.220
332.6	8.867	65.568	64.651	.305	-30.176	-36.860	24.220
400	8.915	67.209	64.947	.905	-30.370	-38.202	20.872
500	8.955	69.203	65.607	1.798	-30.826	-40.113	17.533
582	8.978	70.564	66.212	2.533	-31.416	-41.592	15.618
600	8.983	70.838	66.346	2.695	-31.489	-41.906	15.264
700	9.005	72.225	67.089	3.595	-31.950	-43.607	13.615
768	9.018	73.060	67.581	4.207	-32.324	-44.721	12.726
800	9.024	73.428	67.808	4.496	-32.502	-45.234	12.357
900	9.041	74.492	68.493	5.399	-33.028	-46.795	11.363
1000	9.056	75.445	69.141	6.304	-33.545	-48.297	10.555
1002	9.056	75.463	69.154	6.322	-33.556	-48.327	10.541
1002	9.056	75.463	69.154	6.322	-35.408	-48.327	10.541
1100	9.071	76.309	69.754	7.211	-35.961	-49.563	9.847
1200	9.086	77.099	70.333	8.119	-36.496	-50.775	9.247
1300	9.100	77.827	70.882	9.028	-37.010	-51.944	8.733
1400	9.115	78.502	71.403	9.938	-37.523	-53.076	8.285
1500	9.130	79.131	71.897	10.851	-38.034	-54.166	7.892
1600	9.146	79.721	72.368	11.764	-38.546	-55.226	7.543
1700	9.164	80.276	72.817	12.680	-39.055	-56.253	7.232
1800	9.184	80.800	73.246	13.597	-39.563	-57.251	6.951
1900	9.208	81.298	73.657	14.517	-40.069	-58.219	6.697
2000	9.235	81.771	74.052	15.439	-40.574	-59.163	6.465

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.
1002 K, melting point of Ba; ΔH° = 1.852 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.933 + 0.136\times10^{-3}T - 0.117\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.933\times10^{-3}T + 0.068\times10^{-6}T^2 + 0.117\times10^{2}T^{-1} - 2.709$

BaBr(g) - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -29.348 + 9.610\times10^{-3}T - 18.132\times10^{-6}T^2 + 505.200T^{-1}$

$\Delta Gf^\circ = -29.348 - 9.610\times10^{-3}T\ln T + 18.132\times10^{-6}T^2 + 252.600T^{-1} + 24.905\times10^{-3}T$

332.6-582 K: $\Delta Hf^\circ = -34.348 + 14.191\times10^{-3}T - 18.209\times10^{-6}T^2 + 489.500T^{-1}$

$\Delta Gf^\circ = -34.348 - 14.191\times10^{-3}T\ln T + 18.209\times10^{-6}T^2 + 244.750T^{-1} + 66.583\times10^{-3}T$

582-768 K: $\Delta Hf^\circ = -30.827 + 1.951\times10^{-3}T - 5.069\times10^{-6}T^2 - 4.000T^{-1}$

$\Delta Gf^\circ = -30.827 - 1.951\times10^{-3}T\ln T + 5.069\times10^{-6}T^2 - 2.000T^{-1} - 9.016\times10^{-3}T$

768-1002 K: $\Delta Hf^\circ = -27.872 - 6.191\times10^{-3}T + 0.521\times10^{-6}T^2 - 4.400T^{-1}$

$\Delta Gf^\circ = -27.872 + 6.191\times10^{-3}T\ln T - 0.521\times10^{-6}T^2 - 2.200T^{-1} - 62.665\times10^{-3}T$

1002-2000 K: $\Delta Hf^\circ = -35.126 - 2.124\times10^{-3}T - 0.609\times10^{-6}T^2 + 2461.900T^{-1}$

$\Delta Gf^\circ = -35.126 + 2.124\times10^{-3}T\ln T + 0.609\times10^{-6}T^2 + 1230.950T^{-1} - 29.684\times10^{-3}T$

Source: Data from Chase (26).

$BaBr_2$(c,l)

Barium Dibromide

[Formation: Ba(c,l) + Br_2(l,g) = $BaBr_2$(c,l)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	18.380	35.000	35.000	0	-181.000	-176.141	129.113
300	18.395	35.114	35.001	.034	-181.011	-176.110	128.294
332.6	18.620	37.023	35.107	.637	-181.221	-175.567	115.363
332.6	18.620	37.023	35.107	.637	-188.286	-175.567	115.363
400	19.085	40.506	35.731	1.910	-188.103	-173.014	94.529
500	19.612	44.823	37.131	3.846	-187.957	-169.262	73.984
582	19.992	47.831	38.431	5.470	-188.021	-166.193	62.407
600	20.075	48.441	38.723	5.831	-187.975	-165.519	60.289
700	20.508	51.568	40.339	7.860	-187.754	-161.795	50.514
768	20.792	53.483	41.419	9.265	-187.640	-159.278	45.325
800	20.925	54.334	41.919	9.932	-187.583	-158.097	43.190
900	21.332	56.822	43.439	12.045	-187.348	-154.426	37.499
1000	21.734	59.091	44.893	14.198	-187.067	-150.784	32.953
1002	21.742	59.134	44.921	14.241	-187.062	-150.712	32.872
1002	21.742	59.134	44.921	14.241	-188.914	-150.712	32.872
1100	22.132	61.181	46.280	16.391	-188.648	-146.987	29.203
1130	22.251	61.778	46.683	17.057	-188.553	-145.851	28.208
1130	23.689	68.645	46.683	24.817	-180.793	-145.851	28.208
1200	23.981	70.078	48.006	26.486	-180.447	-143.697	26.170
1300	24.398	72.014	49.779	28.905	-179.904	-140.656	23.646
1400	24.816	73.837	51.433	31.366	-179.319	-137.658	21.489
1500	25.233	75.564	52.985	33.868	-178.695	-134.705	19.626
1600	25.650	77.205	54.448	36.412	-178.030	-131.792	18.002
1700	26.068	78.773	55.833	38.998	-177.324	-128.925	16.574
1800	26.485	80.275	57.149	41.626	-176.577	-126.100	15.310
1900	26.902	81.718	58.405	44.295	-175.790	-123.314	14.184
2000	27.320	83.108	59.605	47.006	-174.963	-120.575	13.176

*Heat capacity at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
582 K, α - β transition point of Ba; $\Delta H°$ = 0 kcal/mol.
768 K, β - γ transition point of Ba; $\Delta H°$ = 0 kcal/mol.
1002 K, melting point of Ba; $\Delta H°$ = 1.852 kcal/mol.
1130 K, melting point of $BaBr_2$; $\Delta H°$ = 7.760 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1130 K: $Cp° = 17.930 + 3.866\times10^{-3}T - 0.625\times10^{5}T^{-2}$

$H°- H°_{298} = 17.930\times10^{-3}T + 1.933\times10^{-6}T^{2} + 0.625\times10^{2}T^{-1} - 5.727$

1130-2000 K: $Cp° = 19.008 + 4.158\times10^{-3}T - 0.210\times10^{5}T^{-2}$

$H°- H°_{298} = 19.008\times10^{-3}T + 2.079\times10^{-6}T^{2} + 0.210\times10^{2}T^{-1} + 0.665$

$BaBr_2$(c,l) - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -184.274 + 9.562\times10^{-3}T - 16.217\times10^{-6}T^2 + 556.000T^{-1}$

$\Delta Gf^\circ = -184.274 - 9.562\times10^{-3}T\ln T + 16.217\times10^{-6}T^2 + 278.000T^{-1} + 73.797\times10^{-3}T$

332.6-582 K: $\Delta Hf^\circ = -194.275 + 18.723\times10^{-3}T - 16.372\times10^{-6}T^2 + 524.600T^{-1}$

$\Delta Gf^\circ = -194.275 - 18.723\times10^{-3}T\ln T + 16.372\times10^{-6}T^2 + 262.300T^{-1} + 157.152\times10^{-3}T$

582-768 K: $\Delta Hf^\circ = -190.754 + 6.483\times10^{-3}T - 3.232\times10^{-6}T^2 + 31.100T^{-1}$

$\Delta Gf^\circ = -190.754 - 6.483\times10^{-3}T\ln T + 3.232\times10^{-6}T^2 + 15.550T^{-1} + 81.553\times10^{-3}T$

768-1002 K: $\Delta Hf^\circ = -187.798 - 1.659\times10^{-3}T + 2.359\times10^{-6}T^2 + 30.700T^{-1}$

$\Delta Gf^\circ = -187.798 + 1.659\times10^{-3}T\ln T - 2.359\times10^{-6}T^2 + 15.350T^{-1} + 27.904\times10^{-3}T$

1002-1130 K: $\Delta Hf^\circ = -195.052 + 2.408\times10^{-3}T + 1.229\times10^{-6}T^2 + 2497.000T^{-1}$

$\Delta Gf^\circ = -195.052 - 2.408\times10^{-3}T\ln T - 1.229\times10^{-6}T^2 + 1248.500T^{-1} + 60.885\times10^{-3}T$

1130-2000 K: $\Delta Hf^\circ = -188.660 + 3.486\times10^{-3}T + 1.375\times10^{-6}T^2 + 2455.500T^{-1}$

$\Delta Gf^\circ = -188.660 - 3.486\times10^{-3}T\ln T - 1.375\times10^{-6}T^2 + 1227.750T^{-1} + 62.988\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Parker (187). Heat capacity at 298 K estimated. Other data based on Efremova (73).

$BaBr_2(g)$

Barium Dibromide (ideal gas)

[Formation: $Ba(c,l) + Br_2(l,g) = BaBr_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	13.630	81.729	81.729	0	-105.000	-114.073	83.617
300	13.633	81.813	81.730	.025	-105.020	-114.129	83.142
332.6	13.671	83.221	81.808	.470	-105.388	-115.100	75.630
332.6	13.671	83.221	81.808	.470	-112.453	-115.100	75.630
400	13.751	85.754	82.266	1.395	-112.618	-115.628	63.175
500	13.808	88.829	83.281	2.774	-113.029	-116.337	50.850
582	13.833	90.928	84.215	3.907	-113.585	-116.839	43.874
600	13.839	91.349	84.422	4.156	-113.650	-116.939	42.594
700	13.857	93.484	85.568	5.541	-114.073	-117.455	36.671
768	13.866	94.769	86.327	6.483	-114.421	-117.767	33.513
800	13.870	95.335	86.676	6.927	-114.588	-117.903	32.209
900	13.878	96.969	87.730	8.315	-115.078	-118.288	28.724
1000	13.884	98.432	88.729	9.703	-115.562	-118.620	25.924
1002	13.884	98.460	88.748	9.731	-115.572	-118.626	25.874
1002	13.884	98.460	88.748	9.731	-117.424	-118.626	25.874
1100	13.889	99.756	89.673	11.091	-117.948	-118.719	23.587
1200	13.892	100.964	90.564	12.480	-118.453	-118.766	21.630
1300	13.895	102.076	91.407	13.870	-118.939	-118.771	19.967
1400	13.897	103.106	92.207	15.259	-119.426	-118.741	18.536
1500	13.899	104.065	92.966	16.649	-119.914	-118.675	17.291
1600	13.900	104.962	93.688	18.039	-120.403	-118.576	16.196
1700	13.901	105.805	94.376	19.429	-120.893	-118.448	15.227
1800	13.902	106.599	95.033	20.819	-121.384	-118.290	14.362
1900	13.903	107.351	95.662	22.210	-121.875	-118.102	13.585
2000	13.904	108.064	96.264	23.600	-122.369	-117.893	12.883

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
582 K, α - β transition point of Ba; $\Delta H°$ = 0 kcal/mol.
768 K, β - γ transition point of Ba; $\Delta H°$ = 0 kcal/mol.
1002 K, melting point of Ba; $\Delta H°$ = 1.852 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.907 + 0.002\times10^{-3}T - 0.246\times10^{5}T^{-2}$

$H°- H°_{298} = 13.907\times10^{-3}T + 0.001\times10^{-6}T^{2} + 0.246\times10^{2}T^{-1} - 4.229$

$BaBr_2(g)$ - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -106.776 + 5.539\times10^{-3}T - 18.149\times10^{-6}T^2 + 518.100T^{-1}$

$\Delta Gf^\circ = -106.776 - 5.539\times10^{-3}T\ln T + 18.149\times10^{-6}T^2 + 259.050T^{-1} - 1.242\times10^{-3}T$

332.6-582 K: $\Delta Hf^\circ = -116.776 + 14.700\times10^{-3}T - 18.304\times10^{-6}T^2 + 486.700T^{-1}$

$\Delta Gf^\circ = -116.776 - 14.700\times10^{-3}T\ln T + 18.304\times10^{-6}T^2 + 243.350T^{-1} + 82.113\times10^{-3}T$

582-768 K: $\Delta Hf^\circ = -113.255 + 2.460\times10^{-3}T - 5.164\times10^{-6}T^2 - 6.800T^{-1}$

$\Delta Gf^\circ = -113.255 - 2.460\times10^{-3}T\ln T + 5.164\times10^{-6}T^2 - 3.400T^{-1} + 6.514\times10^{-3}T$

768-1002 K: $\Delta Hf^\circ = -110.300 - 5.682\times10^{-3}T + 0.427\times10^{-6}T^2 - 7.200T^{-1}$

$\Delta Gf^\circ = -110.300 + 5.682\times10^{-3}T\ln T - 0.427\times10^{-6}T^2 - 3.600T^{-1} - 47.134\times10^{-3}T$

1002-2000 K: $\Delta Hf^\circ = -117.554 - 1.615\times10^{-3}T - 0.703\times10^{-6}T^2 + 2459.100T^{-1}$

$\Delta Gf^\circ = -117.554 + 1.615\times10^{-3}T\ln T + 0.703\times10^{-6}T^2 + 1229.550T^{-1} - 14.153\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (187). Other data from Chase (26) who estimated some molecular constants.

BaCl(g)

Barium Monochloride (ideal gas)

[Formation: $Ba(c,l) + 0.5Cl_2(g) = BaCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.708	61.790	61.790	0	-34.000	-40.031	29.343
300	8.712	61.844	61.791	.016	-34.004	-40.068	29.189
400	8.837	64.370	62.135	.894	-34.266	-42.057	22.978
500	8.904	66.349	62.785	1.782	-34.713	-43.956	19.213
582	8.940	67.705	63.387	2.513	-35.299	-45.430	17.060
600	8.948	67.977	63.520	2.674	-35.370	-45.742	16.661
700	8.979	69.359	64.258	3.571	-35.827	-47.436	14.810
768	8.997	70.192	64.746	4.182	-36.200	-48.546	13.815
800	9.005	70.559	64.971	4.470	-36.378	-49.058	13.402
900	9.026	71.621	65.652	5.372	-36.900	-50.611	12.290
1000	9.045	72.573	66.298	6.275	-37.416	-52.107	11.388
1002	9.045	72.591	66.311	6.293	-37.426	-52.137	11.372
1002	9.045	72.591	66.311	6.293	-39.278	-52.137	11.372
1100	9.063	73.436	66.908	7.181	-39.830	-53.367	10.603
1200	9.081	74.225	67.485	8.088	-40.364	-54.574	9.939
1300	9.099	74.953	68.032	8.997	-40.877	-55.737	9.370
1400	9.119	75.628	68.551	9.908	-41.388	-56.862	8.876
1500	9.142	76.258	69.044	10.821	-41.898	-57.949	8.443
1600	9.169	76.849	69.514	11.736	-42.407	-59.003	8.059
1700	9.201	77.406	69.962	12.655	-42.913	-60.024	7.716
1800	9.238	77.933	70.390	13.577	-43.416	-61.017	7.408
1900	9.282	78.433	70.800	14.502	-43.917	-61.979	7.129
2000	9.332	78.911	71.195	15.433	-44.414	-62.919	6.875

Phase changes: 582 K, α - β transition point of Ba; $\Delta H° = 0$ kcal/mol.
768 K, β - γ transition point of Ba; $\Delta H° = 0$ kcal/mol.
1002 K, melting point of Ba; $\Delta H° = 1.852$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.908 + 0.168\times10^{-3}T - 0.222\times10^{5}T^{-2}$

$H°- H°_{298} = 8.908\times10^{-3}T + 0.084\times10^{-6}T^{2} + 0.222\times10^{2}T^{-1} - 2.738$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf° = -38.235 + 14.217\times10^{-3}T - 18.210\times10^{-6}T^{2} + 481.550T^{-1}$

$\Delta Gf° = -38.235 - 14.217\times10^{-3}T\ln T + 18.210\times10^{-6}T^{2} + 240.775T^{-1} + 66.846\times10^{-3}T$

582-768 K: $\Delta Hf° = -34.715 + 1.977\times10^{-3}T - 5.070\times10^{-6}T^{2} - 11.950T^{-1}$

$\Delta Gf° = -34.715 - 1.977\times10^{-3}T\ln T + 5.070\times10^{-6}T^{2} - 5.975T^{-1} - 8.753\times10^{-3}T$

768-1002 K: $\Delta Hf° = -31.759 - 6.165\times10^{-3}T + 0.521\times10^{-6}T^{2} - 12.350T^{-1}$

$\Delta Gf° = -31.759 + 6.165\times10^{-3}T\ln T - 0.521\times10^{-6}T^{2} - 6.175T^{-1} - 62.401\times10^{-3}T$

1002-2000 K: $\Delta Hf° = -39.013 - 2.098\times10^{-3}T - 0.609\times10^{-6}T^{2} + 2453.950T^{-1}$

$\Delta Gf° = -39.013 + 2.098\times10^{-3}T\ln T + 0.609\times10^{-6}T^{2} + 1226.975T^{-1} - 29.420\times10^{-3}T$

Source: Data from Chase (26).

$BaCl_2(c,l)$
Barium Dichloride
[Formation: $Ba(c,l) + Cl_2(g) = BaCl_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	17.960	29.560	29.560	0	-205.200	-193.677	141.967
300	17.976	29.671	29.561	.033	-205.194	-193.605	141.040
400	18.526	34.926	30.273	1.861	-204.922	-189.790	103.695
500	18.861	39.097	31.635	3.731	-204.813	-186.023	81.310
582	19.133	41.981	32.895	5.288	-204.929	-182.936	68.694
600	19.193	42.565	33.177	5.633	-204.895	-182.256	66.386
700	19.597	45.552	34.735	7.572	-204.749	-178.495	55.728
768	19.944	47.384	35.775	8.915	-204.690	-175.948	50.069
800	20.107	48.201	36.256	9.556	-204.657	-174.751	47.739
900	20.739	50.605	37.718	11.598	-204.484	-171.022	41.529
1000	21.500	52.828	39.119	13.709	-204.239	-167.317	36.567
1002	21.518	52.871	39.146	13.752	-204.234	-167.243	36.478
1002	21.518	52.871	39.146	13.752	-206.086	-167.243	36.478
1100	22.395	54.918	40.462	15.902	-205.815	-163.456	32.475
1198	23.404	56.872	41.726	18.145	-205.425	-159.701	29.134
1198	29.600	60.248	41.726	22.190	-201.380	-159.701	29.134
1200	29.600	60.297	41.756	22.249	-201.359	-159.630	29.072
1235	29.600	61.148	42.294	23.285	-200.980	-158.419	28.034
1235	25.980	64.241	42.294	27.105	-197.160	-158.419	28.034
1300	25.980	65.574	43.425	28.794	-196.687	-156.391	26.291
1400*	25.980	67.499	45.076	31.392	-195.963	-153.319	23.934
1500	25.980	69.291	46.631	33.990	-195.241	-150.297	21.898
1600	25.980	70.968	48.101	36.588	-194.521	-147.324	20.123
1700	25.980	72.543	49.492	39.186	-193.802	-144.395	18.563
1800	25.980	74.028	50.815	41.784	-193.085	-141.511	17.182
1900	25.980	75.433	52.074	44.382	-192.369	-138.664	15.950
2000	25.980	76.765	53.275	46.980	-191.656	-135.856	14.845

*Data above 1400 K extrapolated.

Phase changes: 582 K, α - β transition point of Ba; $\Delta H°$ = 0 kcal/mol.
768 K, β - γ transition point of Ba; $\Delta H°$ = 0 kcal/mol.
1002 K, melting point of Ba; $\Delta H°$ = 1.852 kcal/mol.
1198 K, α - β transition point of $BaCl_2$; $\Delta H°$ = 4.045 kcal/mol.
1235 K, melting point of $BaCl_2$; $\Delta H°$ = 3.820 kcal/mol.

$BaCl_2$(c,l) - Continued

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1198 K: $Cp^\circ = 15.862 + 5.610\times10^{-3}T + 0.378\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 15.862\times10^{-3}T + 2.805\times10^{-6}T^2 - 0.378\times10^{2}T^{-1} - 4.852$

1198-1235 K: $Cp^\circ = 29.600$

$H^\circ - H^\circ_{298} = 29.600\times10^{-3}T - 13.271$

1235-2000 K: $Cp^\circ = 25.980$

$H^\circ - H^\circ_{298} = 25.980\times10^{-3}T - 4.980$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf^\circ = -210.115 + 16.758\times10^{-3}T - 15.533\times10^{-6}T^2 + 387.400T^{-1}$

$\Delta Gf^\circ = -210.115 - 16.758\times10^{-3}T\ln T + 15.533\times10^{-6}T^2 + 193.700T^{-1} + 143.803\times10^{-3}T$

582-768 K: $\Delta Hf^\circ = -206.594 + 4.518\times10^{-3}T - 2.393\times10^{-6}T^2 - 106.100T^{-1}$

$\Delta Gf^\circ = -206.594 - 4.518\times10^{-3}T\ln T + 2.393\times10^{-6}T^2 - 53.050T^{-1} + 68.204\times10^{-3}T$

768-1002 K: $\Delta Hf^\circ = -203.638 - 3.624\times10^{-3}T + 3.198\times10^{-6}T^2 - 106.500T^{-1}$

$\Delta Gf^\circ = -203.638 + 3.624\times10^{-3}T\ln T - 3.198\times10^{-6}T^2 - 53.250T^{-1} + 14.556\times10^{-3}T$

1002-1198 K: $\Delta Hf^\circ = -210.892 + 0.443\times10^{-3}T + 2.068\times10^{-6}T^2 + 2359.800T^{-1}$

$\Delta Gf^\circ = -210.892 - 0.443\times10^{-3}T\ln T - 2.068\times10^{-6}T^2 + 1179.900T^{-1} + 47.537\times10^{-3}T$

1198-1235 K: $\Delta Hf^\circ = -219.311 + 14.181\times10^{-3}T - 0.737\times10^{-6}T^2 + 2397.600T^{-1}$

$\Delta Gf^\circ = -219.311 - 14.181\times10^{-3}T\ln T + 0.737\times10^{-6}T^2 + 1198.800T^{-1} + 148.571\times10^{-3}T$

1235-2000 K: $\Delta Hf^\circ = -211.021 + 10.561\times10^{-3}T - 0.737\times10^{-6}T^2 + 2397.600T^{-1}$

$\Delta Gf^\circ = -211.021 - 10.561\times10^{-3}T\ln T + 0.737\times10^{-6}T^2 + 1198.800T^{-1} + 116.088\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (187). Low-temperature heat capacities and entropy at 298 K from Goodman (91). High-temperature data based on Gardner (87).

$BaCl_2(g)$

Barium Dichloride (ideal gas)

[Formation: $Ba(c,l) + Cl_2(g) = BaCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	13.422	77.826	77.826	0	-119.200	-122.068	89.477
300	13.428	77.909	77.826	.025	-119.202	-122.085	88.938
400	13.630	81.803	78.355	1.379	-119.404	-123.022	67.215
500	13.728	84.856	79.362	2.747	-119.797	-123.886	54.150
582	13.773	86.944	80.286	3.875	-120.342	-124.517	46.758
600	13.783	87.364	80.492	4.123	-120.405	-124.645	45.401
700	13.816	89.492	81.631	5.503	-120.818	-125.322	39.127
768	13.831	90.773	82.384	6.443	-121.162	-125.743	35.782
800	13.838	91.338	82.730	6.886	-121.327	-125.931	34.402
900	13.853	92.969	83.779	8.271	-121.811	-126.477	30.712
1000	13.864	94.429	84.773	9.656	-122.292	-126.971	27.749
1002	13.864	94.457	84.792	9.684	-122.302	-126.981	27.696
1002	13.864	94.457	84.792	9.684	-124.154	-126.981	27.696
1100	13.872	95.751	85.712	11.043	-124.674	-127.231	25.278
1200	13.878	96.958	86.599	12.431	-125.177	-127.441	23.210
1300	13.883	98.069	87.439	13.819	-125.662	-127.609	21.453
1400	13.886	99.098	88.236	15.207	-126.148	-127.743	19.941
1500	13.889	100.056	88.992	16.596	-126.635	-127.838	18.626
1600	13.892	100.953	89.712	17.985	-127.124	-127.903	17.471
1700	13.894	101.795	90.399	19.374	-127.614	-127.935	16.447
1800	13.896	102.589	91.053	20.764	-128.105	-127.941	15.534
1900	13.897	103.340	91.680	22.154	-128.597	-127.915	14.713
2000	13.898	104.053	92.282	23.543	-129.093	-127.869	13.973

Phase changes: 582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.
1002 K, melting point of Ba; ΔH° = 1.852 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.894 + 0.010\times10^{-3}T - 0.422\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.894\times10^{-3}T + 0.005\times10^{-6}T^2 + 0.422\times10^{2}T^{-1} - 4.284$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf^\circ = -123.548 + 14.790\times10^{-3}T - 18.333\times10^{-6}T^2 + 467.400T^{-1}$

$\Delta Gf^\circ = -123.548 - 14.790\times10^{-3}T\ln T + 18.333\times10^{-6}T^2 + 233.700T^{-1} + 81.136\times10^{-3}T$

582-768 K: $\Delta Hf^\circ = -120.027 + 2.550\times10^{-3}T - 5.193\times10^{-6}T^2 - 26.100T^{-1}$

$\Delta Gf^\circ = -120.027 - 2.550\times10^{-3}T\ln T + 5.193\times10^{-6}T^2 - 13.050T^{-1} + 5.537\times10^{-3}T$

768-1002 K: $\Delta Hf^\circ = -117.071 - 5.592\times10^{-3}T + 0.398\times10^{-6}T^2 - 26.500T^{-1}$

$\Delta Gf^\circ = -117.071 + 5.592\times10^{-3}T\ln T - 0.398\times10^{-6}T^2 - 13.250T^{-1} - 48.111\times10^{-3}T$

1002-2000 K: $\Delta Hf^\circ = -124.325 - 1.525\times10^{-3}T - 0.732\times10^{-6}T^2 + 2439.800T^{-1}$

$\Delta Gf^\circ = -124.325 + 1.525\times10^{-3}T\ln T + 0.732\times10^{-6}T^2 + 1219.900T^{-1} - 15.130\times10^{-3}T$

Source: Data from Chase (27).

BaF(g)

Barium Monofluoride (ideal gas)

[Formation: $Ba(c,l) + 0.5F_2(g) = BaF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	8.305	58.823	58.823	0	-77.000	-82.869	60.744
300	8.312	58.874	58.824	.015	-77.004	-82.905	60.395
400	8.571	61.305	59.153	.861	-77.269	-84.838	46.353
500	8.716	63.235	59.783	1.726	-77.714	-86.684	37.889
582	8.789	64.564	60.365	2.444	-78.296	-88.113	33.087
600	8.805	64.832	60.495	2.602	-78.368	-88.415	32.205
700	8.864	66.194	61.214	3.486	-78.823	-90.055	28.116
768	8.893	67.018	61.692	4.090	-79.193	-91.129	25.932
800	8.907	67.381	61.912	4.375	-79.370	-91.622	25.030
900	8.940	68.432	62.580	5.267	-79.893	-93.123	22.613
1000	8.967	69.375	63.213	6.162	-80.410	-94.565	20.667
1002	8.967	69.393	63.225	6.180	-80.421	-94.594	20.632
1002	8.967	69.393	63.225	6.180	-82.273	-94.594	20.632
1100	8.989	70.231	63.813	7.060	-82.827	-95.772	19.028
1200	9.009	71.014	64.381	7.960	-83.364	-96.925	17.652
1300	9.027	71.736	64.919	8.862	-83.880	-98.033	16.481
1400	9.044	72.405	65.430	9.765	-84.397	-99.104	15.471
1500	9.062	73.030	65.916	10.671	-84.913	-100.135	14.590
1600	9.081	73.615	66.379	11.578	-85.428	-101.132	13.814
1700	9.102	74.167	66.822	12.487	-85.944	-102.099	13.126
1800	9.125	74.687	67.244	13.398	-86.459	-103.035	12.510
1900	9.152	75.181	67.648	14.312	-86.971	-103.940	11.956
2000	9.183	75.652	68.037	15.229	-87.482	-104.822	11.454

Phase changes: 582 K, α - β transition point of Ba; $\Delta H° = 0$ kcal/mol.
768 K, β - γ transition point of Ba; $\Delta H° = 0$ kcal/mol.
1002 K, melting point of Ba; $\Delta H° = 1.852$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.855 + 0.158\times10^{-3}T - 0.530\times10^{5}T^{-2}$

$H°-H°_{298} = 8.855\times10^{-3}T + 0.079\times10^{-6}T^2 + 0.530\times10^{2}T^{-1} - 2.825$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf° = -81.312 + 14.324\times10^{-3}T - 18.258\times10^{-6}T^2 + 496.250T^{-1}$

$\Delta Gf° = -81.312 - 14.324\times10^{-3}T\ln T + 18.258\times10^{-6}T^2 + 248.125T^{-1} + 68.157\times10^{-3}T$

582-768 K: $\Delta Hf° = -77.791 + 2.084\times10^{-3}T - 5.118\times10^{-6}T^2 + 2.750T^{-1}$

$\Delta Gf° = -77.791 - 2.084\times10^{-3}T\ln T + 5.118\times10^{-6}T^2 + 1.375T^{-1} - 7.442\times10^{-3}T$

768-1002 K: $\Delta Hf° = -74.835 - 6.058\times10^{-3}T + 0.473\times10^{-6}T^2 + 2.350T^{-1}$

$\Delta Gf° = -74.835 + 6.058\times10^{-3}T\ln T - 0.473\times10^{-6}T^2 + 1.175T^{-1} - 61.091\times10^{-3}T$

1002-2000 K: $\Delta Hf° = -82.089 - 1.991\times10^{-3}T - 0.657\times10^{-6}T^2 + 2468.650T^{-1}$

$\Delta Gf° = -82.089 + 1.991\times10^{-3}T\ln T + 0.657\times10^{-6}T^2 + 1234.325T^{-1} - 28.110\times10^{-3}T$

Source: Data from Chase (27).

BaF_2(c,l)

Barium Difluoride

[Formation: Ba(c,l) + F_2(g) = BaF_2(c,l)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	17.181	23.030	23.030	0	-290.500	-278.475	204.125
300	17.198	23.136	23.030	.032	-290.494	-278.400	202.812
400	17.854	28.180	23.715	1.786	-290.235	-274.414	149.931
500	18.516	32.233	25.025	3.604	-290.129	-270.475	118.223
582	19.074	35.087	26.246	5.146	-290.228	-267.247	100.354
600	19.197	35.670	26.520	5.490	-290.188	-266.537	97.085
700	19.760	38.674	28.047	7.439	-290.002	-262.611	81.990
768	20.093	40.521	29.069	8.795	-289.914	-259.954	73.974
800	20.249	41.344	29.544	9.440	-289.869	-258.707	70.674
900	20.971	43.766	30.992	11.497	-289.662	-254.822	61.878
1000	22.533	46.045	32.384	13.661	-289.350	-250.968	54.848
1002	22.599	46.090	32.411	13.706	-289.342	-250.891	54.722
1002	22.599	46.090	32.411	13.706	-291.194	-250.891	54.722
1100	25.850	48.330	33.729	16.061	-290.708	-246.969	49.068
1200	32.153	50.823	35.047	18.931	-289.720	-243.032	44.262
1300	42.989	53.788	36.370	22.643	-287.874	-239.206	40.214
1310	44.391	54.123	36.505	23.080	-287.624	-238.833	39.844
1310	28.240	54.123	36.505	23.080	-287.624	-238.833	39.844
1400	28.240	55.999	37.698	25.621	-286.766	-235.512	36.765
1480	28.240	57.569	38.731	27.880	-286.005	-232.605	34.348
1480	17.013	57.920	38.731	28.400	-285.485	-232.605	34.348
1500	19.885	58.167	38.988	28.769	-285.491	-231.888	33.786
1600	34.244	59.909	40.237	31.475	-284.661	-228.335	31.189
1640	39.987	60.825	40.728	32.960	-283.927	-226.934	30.241
1640	23.700	63.874	40.728	37.960	-278.927	-226.934	30.241
1700	23.700	64.726	41.560	39.382	-278.632	-225.038	28.930
1800	23.700	66.080	42.884	41.752	-278.144	-221.899	26.942
1900	23.700	67.362	44.140	44.122	-277.657	-218.787	25.166
2000	23.700	68.577	45.331	46.492	-277.174	-215.702	23.571

Phase changes: 582 K, α - β transition point of Ba; $\Delta H°$ = 0 kcal/mol.
768 K, β - γ transition point of Ba; $\Delta H°$ = 0 kcal/mol.
1002 K, melting point of Ba; $\Delta H°$ = 1.852 kcal/mol.
1310 K, α - β transition point of BaF_2; $\Delta H°$ = 0 kcal/mol.
1480 K, β - γ transition point of BaF_2; $\Delta H°$ = 0.520 kcal/mol.
1640 K, melting point of BaF_2; $\Delta H°$ = 5.000 kcal/mol.

BaF_2(c,l) - Continued

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1310 K: $Cp^\circ = 6.938 + 18.392\times10^{-3}T + 4.231\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 6.938\times10^{-3}T + 9.196\times10^{-6}T^2 - 4.231\times10^{2}T^{-1} - 1.467$

1310-1480 K: $Cp^\circ = 28.238$

$H^\circ - H^\circ_{298} = 28.238\times10^{-3}T - 13.912$

1480-1640 K: $Cp^\circ = -195.750 + 143.750\times10^{-3}T$

$H^\circ - H^\circ_{298} = -195.750\times10^{-3}T + 71.875\times10^{-6}T^2 + 160.615$

1640-2000 K: $Cp^\circ = 23.700$

$H^\circ - H^\circ_{298} = 23.700\times10^{-3}T - 0.908$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf^\circ = -292.010 + 8.153\times10^{-3}T - 9.228\times10^{-6}T^2 - 30.100T^{-1}$

$\Delta Gf^\circ = -292.010 - 8.153\times10^{-3}T\ln T + 9.228\times10^{-6}T^2 - 15.050T^{-1} + 89.265\times10^{-3}T$

582-768 K: $\Delta Hf^\circ = -288.489 - 4.087\times10^{-3}T + 3.912\times10^{-6}T^2 - 523.600T^{-1}$

$\Delta Gf^\circ = -288.489 + 4.087\times10^{-3}T\ln T - 3.912\times10^{-6}T^2 - 261.800T^{-1} + 13.665\times10^{-3}T$

768-1002 K: $\Delta Hf^\circ = -285.533 - 12.229\times10^{-3}T + 9.503\times10^{-6}T^2 - 524.000T^{-1}$

$\Delta Gf^\circ = -285.533 + 12.229\times10^{-3}T\ln T - 9.503\times10^{-6}T^2 - 262.000T^{-1} - 39.983\times10^{-3}T$

1002-1310 K: $\Delta Hf^\circ = -292.787 - 8.162\times10^{-3}T + 8.373\times10^{-6}T^2 + 1942.300T^{-1}$

$\Delta Gf^\circ = -292.787 + 8.162\times10^{-3}T\ln T - 8.373\times10^{-6}T^2 + 971.150T^{-1} - 7.002\times10^{-3}T$

1310-1480 K: $\Delta Hf^\circ = -305.232 + 13.138\times10^{-3}T - 0.823\times10^{-6}T^2 + 2365.400T^{-1}$

$\Delta Gf^\circ = -305.232 - 13.138\times10^{-3}T\ln T + 0.823\times10^{-6}T^2 + 1182.700T^{-1} + 143.215\times10^{-3}T$

1480-1640 K: $\Delta Hf^\circ = -130.644 - 210.850\times10^{-3}T + 71.052\times10^{-6}T^2 + 2365.400T^{-1}$

$\Delta Gf^\circ = -130.644 + 210.850\times10^{-3}T\ln T - 71.052\times10^{-6}T^2 + 1182.700T^{-1} - 1503.445\times10^{-3}T$

1640-2000 K: $\Delta Hf^\circ = -292.227 + 8.600\times10^{-3}T - 0.823\times10^{-6}T^2 + 2365.400T^{-1}$

$\Delta Gf^\circ = -292.227 - 8.600\times10^{-3}T\ln T + 0.823\times10^{-6}T^2 + 1182.700T^{-1} + 101.678\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (188). Low-temperature heat capacities and entropy at 298 K based on Pitzer (196). High-temperature data based on Efremova (73).

$BaF_2(g)$

Barium Difluoride (ideal gas)

[Formation: $Ba(c,l) + F_2(g) = BaF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.854	71.985	71.985	0	-192.100	-194.671	142.696
300	12.864	72.064	71.985	.024	-192.102	-194.687	141.827
400	13.277	75.829	72.497	1.333	-192.288	-195.527	106.830
500	13.490	78.817	73.471	2.673	-192.660	-196.298	85.801
582	13.591	80.874	74.373	3.783	-193.190	-196.857	73.922
600	13.613	81.288	74.575	4.028	-193.250	-196.969	71.745
700	13.689	83.392	75.686	5.394	-193.647	-197.559	61.680
768	13.724	84.663	76.427	6.326	-193.983	-197.924	56.323
800	13.740	85.224	76.768	6.765	-194.144	-198.086	54.114
900	13.775	86.844	77.798	8.141	-194.618	-198.548	48.213
1000	13.800	88.297	78.777	9.520	-195.091	-198.961	43.482
1002	13.800	88.325	78.796	9.548	-195.101	-198.969	43.397
1002	13.800	88.325	78.796	9.548	-196.953	-198.969	43.397
1100	13.819	89.613	79.703	10.901	-197.468	-199.140	39.565
1200	13.833	90.816	80.579	12.284	-197.967	-199.270	36.292
1300	13.845	91.924	81.411	13.667	-198.450	-199.359	33.515
1400	13.853	92.950	82.199	15.052	-198.935	-199.412	31.129
1500	13.861	93.906	82.947	16.438	-199.422	-199.428	29.056
1600	13.867	94.801	83.661	17.824	-199.912	-199.413	27.238
1700	13.872	95.642	84.341	19.211	-200.403	-199.366	25.630
1800	13.876	96.435	84.991	20.599	-200.897	-199.291	24.197
1900	13.879	97.185	85.613	21.987	-201.392	-199.186	22.911
2000	13.882	97.897	86.210	23.375	-201.891	-199.059	21.752

Phase changes: 582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.
1002 K, melting point of Ba; ΔH° = 1.852 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.815 + 0.060\times10^{-3}T - 0.870\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.815\times10^{-3}T + 0.030\times10^{-6}T^2 + 0.870\times10^{2}T^{-1} - 4.413$

Formation equations (kcal/mol):

298.15-582 K: $\Delta Hf^\circ = -196.556 + 15.030\times10^{-3}T - 18.394\times10^{-6}T^2 + 480.000T^{-1}$

$\Delta Gf^\circ = -196.556 - 15.030\times10^{-3}T\ln T + 18.394\times10^{-6}T^2 + 240.000T^{-1} + 83.772\times10^{-3}T$

582-768 K: $\Delta Hf^\circ = -193.035 + 2.790\times10^{-3}T - 5.254\times10^{-6}T^2 - 13.500T^{-1}$

$\Delta Gf^\circ = -193.035 - 2.790\times10^{-3}T\ln T + 5.254\times10^{-6}T^2 - 6.750T^{-1} + 8.173\times10^{-3}T$

768-1002 K: $\Delta Hf^\circ = -190.079 - 5.352\times10^{-3}T + 0.337\times10^{-6}T^2 - 13.900T^{-1}$

$\Delta Gf^\circ = -190.079 + 5.352\times10^{-3}T\ln T - 0.337\times10^{-6}T^2 - 6.950T^{-1} - 45.475\times10^{-3}T$

1002-2000 K: $\Delta Hf^\circ = -197.333 - 1.285\times10^{-3}T - 0.793\times10^{-6}T^2 + 2452.400T^{-1}$

$\Delta Gf^\circ = -197.333 + 1.285\times10^{-3}T\ln T + 0.793\times10^{-6}T^2 + 1226.200T^{-1} - 12.494\times10^{-3}T$

Source: Data from Chase (27).

BaI(g)

Barium Monoiodide (ideal gas)

[Formation: $Ba(c,l) + 0.5I_2(c,l,g) = BaI(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.896	66.593	66.593	0	-10.140	-21.409	15.693
300	8.897	66.648	66.595	.016	-10.148	-21.479	15.647
386.8	8.941	68.915	66.870	.791	-10.600	-24.704	13.958
386.8	8.941	68.915	66.870	.791	-12.454	-24.704	13.958
400	8.948	69.215	66.942	.909	-12.567	-25.120	13.725
458.4	8.966	70.436	67.312	1.432	-13.102	-26.915	12.832
458.4	8.966	70.436	67.312	1.432	-18.113	-26.915	12.832
500	8.979	71.215	67.605	1.805	-18.338	-27.703	12.109
582	8.998	72.580	68.210	2.543	-18.929	-29.195	10.963
600	9.002	72.854	68.346	2.705	-19.002	-29.511	10.749
700	9.022	74.244	69.093	3.606	-19.465	-31.229	9.750
768	9.034	75.080	69.586	4.220	-19.839	-32.353	9.207
800	9.039	75.449	69.813	4.509	-20.019	-32.871	8.980
900	9.055	76.515	70.501	5.413	-20.546	-34.447	8.365
1000	9.071	77.470	71.150	6.320	-21.063	-35.964	7.860
1002	9.071	77.488	71.163	6.338	-21.074	-35.994	7.851
1002	9.071	77.488	71.163	6.338	-22.926	-35.994	7.851
1100	9.086	78.335	71.764	7.228	-23.481	-37.244	7.400
1200	9.100	79.126	72.345	8.137	-24.017	-38.472	7.007
1300	9.115	79.855	72.895	9.048	-24.532	-39.654	6.666
1400	9.129	80.531	73.417	9.960	-25.046	-40.800	6.369
1500	9.143	81.162	73.913	10.873	-25.559	-41.908	6.106
1600	9.157	81.752	74.384	11.789	-26.070	-42.979	5.871
1700	9.172	82.308	74.834	12.705	-26.582	-44.021	5.659
1800	9.186	82.832	75.264	13.623	-27.093	-45.032	5.468
1900	9.200	83.329	75.675	14.542	-27.603	-46.014	5.293
2000	9.214	83.802	76.071	15.463	-28.112	-46.972	5.133

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.
1002 K, melting point of Ba; ΔH° = 1.852 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.938 + 0.140\times10^{-3}T - 0.074\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.938\times10^{-3}T + 0.070\times10^{-6}T^2 + 0.074\times10^{2}T^{-1} - 2.696$

BaI(g) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -13.782 + 12.222\times10^{-3}T - 18.926\times10^{-6}T^2 + 500.900T^{-1}$

$\Delta Gf^\circ = -13.782 - 12.222\times10^{-3}T\ln T + 18.926\times10^{-6}T^2 + 250.450T^{-1} + 35.597\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -14.509 + 9.020\times10^{-3}T - 18.180\times10^{-6}T^2 + 500.900T^{-1}$

$\Delta Gf^\circ = -14.509 - 9.020\times10^{-3}T\ln T + 18.180\times10^{-6}T^2 + 250.450T^{-1} + 18.690\times10^{-3}T$

458.4-582 K: $\Delta Hf^\circ = -21.866 + 14.190\times10^{-3}T - 18.214\times10^{-6}T^2 + 493.250T^{-1}$

$\Delta Gf^\circ = -21.866 - 14.190\times10^{-3}T\ln T + 18.214\times10^{-6}T^2 + 246.625T^{-1} + 66.421\times10^{-3}T$

582-768 K: $\Delta Hf^\circ = -18.345 + 1.950\times10^{-3}T - 5.074\times10^{-6}T^2 - 0.250T^{-1}$

$\Delta Gf^\circ = -18.345 - 1.950\times10^{-3}T\ln T + 5.074\times10^{-6}T^2 - 0.125T^{-1} - 9.178\times10^{-3}T$

768-1002 K: $\Delta Hf^\circ = -15.389 - 6.192\times10^{-3}T + 0.517\times10^{-6}T^2 - 0.650T^{-1}$

$\Delta Gf^\circ = -15.389 + 6.192\times10^{-3}T\ln T - 0.517\times10^{-6}T^2 - 0.325T^{-1} - 62.826\times10^{-3}T$

1002-2000 K: $\Delta Hf^\circ = -22.643 - 2.125\times10^{-3}T - 0.613\times10^{-6}T^2 + 2465.650T^{-1}$

$\Delta Gf^\circ = -22.643 + 2.125\times10^{-3}T\ln T + 0.613\times10^{-6}T^2 + 1232.825T^{-1} - 29.845\times10^{-3}T$

Source: Data from Chase (27).

$BaI_2(c,l)$
Barium Diiodide
[Formation: $Ba(c,l) + I_2(c,l,g) = BaI_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH_f°	ΔG_f°	
298.15	18.515	39.470	39.470	0	-143.900	-142.944	104.780
300*	18.526	39.585	39.472	.034	-143.902	-142.938	104.129
386.8	19.032	44.355	40.052	1.664	-144.102	-142.641	80.594
386.8	19.032	44.355	40.052	1.664	-147.811	-142.641	80.594
400	19.109	44.995	40.205	1.916	-147.918	-142.462	77.837
458.4	19.426	47.621	40.984	3.042	-148.412	-141.629	67.523
458.4	19.426	47.621	40.984	3.042	-158.433	-141.629	67.523
500	19.651	49.318	41.608	3.855	-158.405	-140.103	61.238
582	20.062	52.334	42.912	5.483	-158.473	-137.101	51.483
600	20.152	52.946	43.204	5.845	-158.427	-136.440	49.698
700	20.613	56.087	44.824	7.884	-158.202	-132.793	41.459
768	20.899	58.012	45.909	9.295	-158.085	-130.331	37.088
800	21.033	58.868	46.410	9.966	-158.027	-129.176	35.289
900	21.413	61.367	47.935	12.089	-157.787	-125.583	30.495
984	21.701	63.291	49.165	13.900	-157.552	-122.588	27.227
984	27.000	69.734	49.165	20.240	-151.212	-122.588	27.227
1000	27.000	70.169	49.497	20.672	-151.081	-122.123	26.690
1002	27.000	70.223	49.538	20.726	-151.065	-122.065	26.624
1002	27.000	70.223	49.538	20.726	-152.917	-122.065	26.624
1100	27.000	72.743	51.496	23.372	-152.160	-119.084	23.660
1200	27.000	75.092	53.365	26.072	-151.360	-116.112	21.147
1300	27.000	77.253	55.121	28.772	-150.540	-113.207	19.032
1400	27.000	79.254	56.774	31.472	-149.722	-110.367	17.229
1500	27.000	81.117	58.336	34.172	-148.905	-107.584	15.675
1600	27.000	82.860	59.815	36.872	-148.089	-104.855	14.322
1700	27.000	84.496	61.218	39.572	-147.275	-102.177	13.136
1800	27.000	86.040	62.556	42.272	-146.462	-99.550	12.087
1900	27.000	87.499	63.830	44.972	-145.651	-96.964	11.153
2000	27.000	88.884	65.048	47.672	-144.841	-94.423	10.318

*Data 300-984 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.
984 K, melting point of BaI_2; ΔH° = 6.340 kcal/mol.
1002 K, melting point of Ba; ΔH° = 1.852 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-984 K: $C_p^\circ = 17.629 + 4.302\times10^{-3}T - 0.355\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 17.629\times10^{-3}T + 2.151\times10^{-6}T^2 + 0.355\times10^{2}T^{-1} - 5.566$

984-2000 K: $C_p^\circ = 27.000$

$H^\circ - H^\circ_{298} = 27.000\times10^{-3}T - 6.328$

BaI_2(c,l) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -148.426 + 14.475\times10^{-3}T - 17.591\times10^{-6}T^2 + 529.000T^{-1}$

$\Delta Gf^\circ = -148.426 - 14.475\times10^{-3}T\ln T + 17.591\times10^{-6}T^2 + 264.500T^{-1} + 92.640\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -149.881 + 8.071\times10^{-3}T - 16.099\times10^{-6}T^2 + 529.000T^{-1}$

$\Delta Gf^\circ = -149.881 - 8.071\times10^{-3}T\ln T + 16.099\times10^{-6}T^2 + 264.500T^{-1} + 58.824\times10^{-3}T$

458.4-582 K: $\Delta Hf^\circ = -164.595 + 18.411\times10^{-3}T - 16.167\times10^{-6}T^2 + 513.700T^{-1}$

$\Delta Gf^\circ = -164.595 - 18.411\times10^{-3}T\ln T + 16.167\times10^{-6}T^2 + 256.850T^{-1} + 154.287\times10^{-3}T$

582-768 K: $\Delta Hf^\circ = -161.074 + 6.171\times10^{-3}T - 3.027\times10^{-6}T^2 + 20.200T^{-1}$

$\Delta Gf^\circ = -161.074 - 6.171\times10^{-3}T\ln T + 3.027\times10^{-6}T^2 + 10.100T^{-1} + 78.688\times10^{-3}T$

768-984 K: $\Delta Hf^\circ = -158.118 - 1.971\times10^{-3}T + 2.564\times10^{-6}T^2 + 19.800T^{-1}$

$\Delta Gf^\circ = -158.118 + 1.971\times10^{-3}T\ln T - 2.564\times10^{-6}T^2 + 9.900T^{-1} + 25.040\times10^{-3}T$

984-1002 K: $\Delta Hf^\circ = -158.880 + 7.400\times10^{-3}T + 0.413\times10^{-6}T^2 - 15.700T^{-1}$

$\Delta Gf^\circ = -158.880 - 7.400\times10^{-3}T\ln T - 0.413\times10^{-6}T^2 - 7.850T^{-1} + 88.298\times10^{-3}T$

1002-2000 K: $\Delta Hf^\circ = -166.134 + 11.467\times10^{-3}T - 0.717\times10^{-6}T^2 + 2450.600T^{-1}$

$\Delta Gf^\circ = -166.134 - 11.467\times10^{-3}T\ln T + 0.717\times10^{-6}T^2 + 1225.300T^{-1} + 121.279\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (187). Low-temperature heat capacities and entropy at 298 K from Paukov (190). Data estimated between 300 K and 984 K from Dworkin's (66) single reported value at 984 K. Temperature and enthalpy of fusion and heat capacity of liquid also from Dworkin (66).

$BaI_2(g)$

Barium Diiodide (ideal gas)

[Formation: $Ba(c,l) + I_2(c,l,g) = BaI_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	13.734	83.180	83.180	0	-72.400	-84.476	61.922
300	13.736	83.265	83.182	.025	-72.411	-84.551	61.594
386.8	13.801	86.765	83.609	1.221	-73.046	-87.988	49.714
386.8	13.801	86.765	83.609	1.221	-76.755	-87.988	49.714
400	13.811	87.228	83.720	1.403	-76.931	-88.369	48.282
458.4	13.831	89.112	84.290	2.210	-77.744	-89.980	42.899
458.4	13.831	89.112	84.290	2.210	-87.765	-89.980	42.899
500	13.846	90.314	84.742	2.786	-87.974	-90.170	39.413
582	13.862	92.419	85.679	3.922	-88.534	-90.491	33.980
600	13.866	92.841	85.888	4.172	-88.600	-90.550	32.982
700	13.877	94.979	87.038	5.559	-89.027	-90.843	28.362
768	13.882	96.265	87.798	6.503	-89.378	-91.002	25.896
800	13.885	96.832	88.148	6.947	-89.546	-91.066	24.878
900	13.890	98.468	89.206	8.336	-90.040	-91.227	22.153
1000	13.894	99.932	90.207	9.725	-90.528	-91.333	19.961
1002	13.894	99.960	90.226	9.753	-90.538	-91.335	19.921
1002	13.894	99.960	90.226	9.753	-92.390	-91.335	19.921
1100	13.897	101.256	91.151	11.115	-92.917	-91.205	18.121
1200	13.899	102.466	92.045	12.505	-93.427	-91.028	16.578
1300	13.901	103.578	92.890	13.895	-93.917	-90.806	15.266
1400	13.902	104.608	93.690	15.285	-94.409	-90.549	14.135
1500	13.903	105.567	94.450	16.675	-94.902	-90.257	13.150
1600	13.904	106.465	95.174	18.065	-95.396	-89.930	12.284
1700	13.905	107.308	95.863	19.456	-95.891	-89.574	11.515
1800	13.905	108.103	96.522	20.846	-96.388	-89.190	10.829
1900	13.906	108.854	97.150	22.237	-96.886	-88.773	10.211
2000	13.906	109.568	97.755	23.627	-97.386	-88.336	9.653

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
768 K, β - γ transition point of Ba; ΔH° = 0 kcal/mol.
1002 K, melting point of Ba; ΔH° = 1.852 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.907 + 0.002\times10^{-3}T - 0.154\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.907\times10^{-3}T + 0.001\times10^{-6}T^2 + 0.154\times10^{2}T^{-1} - 4.198$

BaI_2(g) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -75.558 + 10.753\times10^{-3}T - 19.741\times10^{-6}T^2 + 508.900T^{-1}$

$\Delta Gf^\circ = -75.558 - 10.753\times10^{-3}T\ln T + 19.741\times10^{-6}T^2 + 254.450T^{-1} + 22.606\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -77.013 + 4.349\times10^{-3}T - 18.249\times10^{-6}T^2 + 508.900T^{-1}$

$\Delta Gf^\circ = -77.013 - 4.349\times10^{-3}T\ln T + 18.249\times10^{-6}T^2 + 254.450T^{-1} - 11.209\times10^{-3}T$

458.4-582 K: $\Delta Hf^\circ = -91.726 + 14.689\times10^{-3}T - 18.317\times10^{-6}T^2 + 493.600T^{-1}$

$\Delta Gf^\circ = -91.726 - 14.689\times10^{-3}T\ln T + 18.317\times10^{-6}T^2 + 246.800T^{-1} + 84.254\times10^{-3}T$

582-768 K: $\Delta Hf^\circ = -88.206 + 2.449\times10^{-3}T - 5.177\times10^{-6}T^2 + 0.100T^{-1}$

$\Delta Gf^\circ = -88.206 - 2.449\times10^{-3}T\ln T + 5.177\times10^{-6}T^2 + 0.050T^{-1} + 8.655\times10^{-3}T$

768-1002 K: $\Delta Hf^\circ = -85.250 - 5.693\times10^{-3}T + 0.414\times10^{-6}T^2 - 0.300T^{-1}$

$\Delta Gf^\circ = -85.250 + 5.693\times10^{-3}T\ln T - 0.414\times10^{-6}T^2 - 0.150T^{-1} - 44.994\times10^{-3}T$

1002-2000 K: $\Delta Hf^\circ = -92.504 - 1.626\times10^{-3}T - 0.716\times10^{-6}T^2 + 2466.000T^{-1}$

$\Delta Gf^\circ = -92.504 + 1.626\times10^{-3}T\ln T + 0.716\times10^{-6}T^2 + 1233.000T^{-1} - 12.013\times10^{-3}T$

Source: Data from Chase (27) who estimated some molecular constants.

BeBr(g)

Beryllium Monobromide (ideal gas)

[Formation: $Be(c,l) + 0.5Br_2(l,g) = BeBr(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	7.791	54.594	54.594	0	28.700	18.523	-13.577
300	7.799	54.642	54.595	.014	28.691	18.459	-13.447
332.6	7.923	55.453	54.640	.270	28.520	17.355	-11.404
332.6	7.923	55.453	54.640	.270	24.987	17.355	-11.404
400	8.178	56.942	54.905	.815	24.935	15.813	-8.640
500	8.424	58.795	55.503	1.646	24.824	13.542	-5.919
600	8.585	60.346	56.184	2.497	24.686	11.303	-4.117
700	8.696	61.678	56.877	3.361	24.528	9.080	-2.835
800	8.776	62.845	57.551	4.235	24.357	6.887	-1.881
900	8.837	63.882	58.198	5.116	24.171	4.718	-1.146
1000	8.884	64.816	58.814	6.002	23.969	2.564	-.560
1100	8.922	65.664	59.399	6.892	23.746	.434	-.086
1200	8.954	66.442	59.954	7.786	23.506	-1.680	.306
1300	8.982	67.160	60.481	8.683	23.244	-3.762	.632
1400	9.006	67.827	60.983	9.582	22.962	-5.829	.910
1500	9.027	68.449	61.460	10.484	22.661	-7.885	1.149
1527	9.032	68.610	61.585	10.728	22.576	-8.428	1.206
1527	9.032	68.610	61.585	10.728	21.965	-8.428	1.206
1560	9.039	68.803	61.735	11.026	21.860	-9.091	1.274
1560	9.039	68.803	61.735	11.026	18.941	-9.091	1.274
1600	9.047	69.032	61.914	11.388	18.839	-9.807	1.340
1700	9.065	69.581	62.350	12.293	18.584	-11.602	1.492
1800	9.083	70.100	62.766	13.201	18.333	-13.375	1.624
1900	9.099	70.591	63.165	14.110	18.082	-15.110	1.738
2000	9.114	71.058	63.548	15.020	17.831	-16.854	1.842

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
1527 K, α - β transition point of Be; ΔH° = 0.611 kcal/mol.
1560 K, melting point of Be; ΔH° = 2.919 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.625 + 0.302\times10^{-3}T - 0.822\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.625\times10^{-3}T + 0.151\times10^{-6}T^2 + 0.822\times10^{2}T^{-1} - 2.861$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = 30.444 - 5.161\times10^{-3}T - 0.761\times10^{-6}T^2 - 40.900T^{-1}$

$\Delta Gf^\circ = 30.444 + 5.161\times10^{-3}T\ln T + 0.761\times10^{-6}T^2 - 20.450T^{-1} - 69.388\times10^{-3}T$

332.6-1527 K: $\Delta Hf^\circ = 25.444 - 0.581\times10^{-3}T - 0.839\times10^{-6}T^2 - 56.600T^{-1}$

$\Delta Gf^\circ = 25.444 + 0.581\times10^{-3}T\ln T + 0.839\times10^{-6}T^2 - 28.300T^{-1} - 27.710\times10^{-3}T$

1527-1560 K: $\Delta Hf^\circ = 27.027 - 3.540\times10^{-3}T + 0.124\times10^{-6}T^2 + 66.500T^{-1}$

$\Delta Gf^\circ = 27.027 + 3.540\times10^{-3}T\ln T - 0.124\times10^{-6}T^2 + 33.250T^{-1} - 48.998\times10^{-3}T$

1560-2000 K: $\Delta Hf^\circ = 23.079 - 2.880\times10^{-3}T + 0.124\times10^{-6}T^2 + 66.500T^{-1}$

$\Delta Gf^\circ = 23.079 + 2.880\times10^{-3}T\ln T - 0.124\times10^{-6}T^2 + 33.250T^{-1} - 41.614\times10^{-3}T$

Source: Data from Chase (26).

$BeBr_2(c)$
Beryllium Dibromide
[Formation: $Be(c) + Br_2(l,g) = BeBr_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	15.780	24.000	24.000	0	-85.000	-80.632	59.104
300	15.810	24.098	24.001	.029	-85.011	-80.606	58.721
332.6	16.159	25.747	24.093	.550	-85.211	-80.117	52.644
332.6	16.159	25.747	24.093	.550	-92.276	-80.117	52.644
400	16.880	28.794	24.634	1.664	-92.054	-77.677	42.440
500	17.880	32.674	25.864	3.405	-91.696	-74.126	32.400
600	18.550	35.996	27.283	5.228	-91.306	-70.643	25.731
700	19.050	38.895	28.739	7.109	-90.893	-67.236	20.992
752	19.250	40.268	29.490	8.105	-90.670	-65.486	19.032

*Data estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
752 K, sublimation point to $BeBr_2(g)$; ΔH°_{298} = 30.2 kcal/mol.
781 ± 15 K, melting point of $BeBr_2$; ΔH° = 2.4 ± 2 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-752 K: $Cp^\circ = 15.231 + 5.922\times10^{-3}T - 1.082\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 15.231\times10^{-3}T + 2.961\times10^{-6}T^2 + 1.082\times10^{2}T^{-1} - 5.167$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -82.870 - 7.601\times10^{-3}T + 2.099\times10^{-6}T^2 - 14.900T^{-1}$
$\Delta Gf^\circ = -82.870 + 7.601\times10^{-3}T\ln T - 2.099\times10^{-6}T^2 - 7.450T^{-1} - 35.092\times10^{-3}T$
332.6-752 K: $\Delta Hf^\circ = -92.871 + 1.560\times10^{-3}T + 1.944\times10^{-6}T^2 - 46.300T^{-1}$
$\Delta Gf^\circ = -92.871 - 1.560\times10^{-3}T\ln T - 1.944\times10^{-6}T^2 - 23.150T^{-1} + 48.263\times10^{-3}T$

Source: Data are those estimated by Chase (26).

$BeBr_2(g)$

Beryllium Dibromide (ideal gas)

[Formation: $Be(c,l) + Br_2(l,g) = BeBr_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.742	65.439	65.439	0	-54.800	-62.787	46.024
300	12.755	65.518	65.439	.024	-54.816	-62.837	45.776
332.6	12.946	66.844	65.512	.443	-55.118	-63.693	41.852
332.6	12.946	66.844	65.512	.443	-62.183	-63.693	41.852
400	13.340	69.272	65.947	1.330	-62.188	-64.002	34.969
500	13.744	72.295	66.923	2.686	-62.215	-64.455	28.173
600	14.023	74.827	68.035	4.075	-62.259	-64.895	23.638
700	14.218	77.005	69.166	5.487	-62.315	-65.335	20.398
800	14.358	78.913	70.267	6.917	-62.378	-65.760	17.964
900	14.461	80.610	71.323	8.358	-62.453	-66.175	16.069
1000	14.537	82.138	72.330	9.808	-62.541	-66.587	14.552
1100	14.596	83.526	73.285	11.265	-62.648	-66.986	13.309
1200	14.643	84.798	74.192	12.727	-62.772	-67.380	12.271
1300	14.679	85.972	75.054	14.193	-62.917	-67.753	11.390
1400	14.709	87.061	75.874	15.662	-63.082	-68.118	10.634
1500	14.733	88.077	76.654	17.135	-63.266	-68.482	9.978
1527	14.738	88.340	76.858	17.533	-63.319	-68.569	9.814
1527	14.738	88.340	76.858	17.533	-63.930	-68.569	9.814
1560	14.745	88.655	77.104	18.019	-63.998	-68.676	9.621
1560	14.745	88.655	77.104	18.019	-66.917	-68.676	9.621
1600	14.753	89.028	77.397	18.609	-66.973	-68.719	9.386
1700	14.769	89.923	78.108	20.085	-67.111	-68.836	8.849
1800	14.784	90.768	78.789	21.563	-67.248	-68.938	8.370
1900	14.796	91.567	79.440	23.042	-67.385	-69.008	7.938
2000	14.806	92.326	80.065	24.522	-67.523	-69.093	7.550

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
1527 K, α - β transition point of Be; ΔH° = 0.611 kcal/mol.
1560 K, melting point of Be; ΔH° = 2.919 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 14.082 + 0.498\times10^{-3}T - 1.323\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.082\times10^{-3}T + 0.249\times10^{-6}T^2 + 1.323\times10^{2}T^{-1} - 4.664$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -52.168 - 8.750\times10^{-3}T - 0.613\times10^{-6}T^2 + 9.200T^{-1}$

$\Delta Gf^\circ = -52.168 + 8.750\times10^{-3}T\ln T + 0.613\times10^{-6}T^2 + 4.600T^{-1} - 85.708\times10^{-3}T$

332.6-1527 K: $\Delta Hf^\circ = -62.168 + 0.411\times10^{-3}T - 0.768\times10^{-6}T^2 - 22.200T^{-1}$

$\Delta Gf^\circ = -62.168 - 0.411\times10^{-3}T\ln T + 0.768\times10^{-6}T^2 - 11.100T^{-1} - 2.353\times10^{-3}T$

1527-1560 K: $\Delta Hf^\circ = -60.584 - 2.548\times10^{-3}T + 0.194\times10^{-6}T^2 + 100.900T^{-1}$

$\Delta Gf^\circ = -60.584 + 2.548\times10^{-3}T\ln T - 0.194\times10^{-6}T^2 + 50.450T^{-1} - 23.640\times10^{-3}T$

1560-2000 K: $\Delta Hf^\circ = -64.533 - 1.888\times10^{-3}T + 0.194\times10^{-6}T^2 + 100.900T^{-1}$

$\Delta Gf^\circ = -64.533 + 1.888\times10^{-3}T\ln T - 0.194\times10^{-6}T^2 + 50.450T^{-1} - 16.256\times10^{-3}T$

Source: Data from Chase (26).

BeCl(g)

Beryllium Monochloride (ideal gas)

[Formation: $Be(c,l) + 0.5Cl_2(g) = BeCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.563	51.984	51.984	0	14.500	7.622	-5.587
300	7.571	52.031	51.984	.014	14.500	7.578	-5.521
400	7.963	54.265	52.285	.792	14.426	5.281	-2.886
500	8.243	56.074	52.868	1.603	14.310	3.005	-1.314
600	8.437	57.595	53.533	2.437	14.165	.761	-.277
700	8.573	58.907	54.210	3.288	14.002	-1.464	.457
800	8.672	60.058	54.869	4.151	13.824	-3.660	1.000
900	8.746	61.084	55.504	5.022	13.632	-5.830	1.416
1000	8.804	62.009	56.109	5.900	13.425	-7.984	1.745
1100	8.850	62.850	56.685	6.782	13.197	-10.116	2.010
1200	8.888	63.622	57.231	7.669	12.951	-12.230	2.227
1300	8.919	64.335	57.750	8.560	12.685	-14.311	2.406
1400	8.947	64.997	58.245	9.453	12.398	-16.376	2.556
1500	8.970	65.615	58.716	10.349	12.092	-18.431	2.685
1527	8.976	65.775	58.839	10.591	12.006	-18.974	2.716
1527	8.976	65.775	58.839	10.591	11.395	-18.974	2.716
1560	8.983	65.966	58.987	10.887	11.287	-19.636	2.751
1560	8.983	65.966	58.987	10.887	8.368	-19.636	2.751
1600	8.992	66.194	59.165	11.247	8.264	-20.351	2.780
1700	9.011	66.740	59.595	12.147	8.006	-22.143	2.847
1800	9.029	67.256	60.007	13.049	7.748	-23.915	2.904
1900	9.045	67.744	60.400	13.953	7.492	-25.647	2.950
2000	9.060	68.208	60.779	14.858	7.236	-27.387	2.993

Phase changes: 1527 K, α - β transition point of Be; $\Delta H° = 0.611$ kcal/mol.
1560 K, melting point of Be; $\Delta H° = 2.919$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.431 + 0.402\times10^{-3}T - 0.878\times10^{5}T^{-2}$

$H°- H°_{298} = 8.431\times10^{-3}T + 0.201\times10^{-6}T^{2} + 0.878\times10^{2}T^{-1} - 2.826$

Formation equations (kcal/mol):

298.15-1527 K: $\Delta Hf° = 15.020 - 0.724\times10^{-3}T - 0.805\times10^{-6}T^{2} - 69.450T^{-1}$

$\Delta Gf° = 15.020 + 0.724\times10^{-3}T\ln T + 0.805\times10^{-6}T^{2} - 34.725T^{-1} - 28.785\times10^{-3}T$

1527-1560 K: $\Delta Hf° = 16.604 - 3.683\times10^{-3}T + 0.157\times10^{-6}T^{2} + 53.650T^{-1}$

$\Delta Gf° = 16.604 + 3.683\times10^{-3}T\ln T - 0.157\times10^{-6}T^{2} + 26.825T^{-1} - 50.073\times10^{-3}T$

1560-2000 K: $\Delta Hf° = 12.655 - 3.023\times10^{-3}T + 0.157\times10^{-6}T^{2} + 53.650T^{-1}$

$\Delta Gf° = 12.655 + 3.023\times10^{-3}T\ln T - 0.157\times10^{-6}T^{2} + 26.825T^{-1} - 42.689\times10^{-3}T$

Source: Data from JANAF (60).

$BeCl_2(\beta,\alpha,l)$

Beryllium Dichloride

[Formation: $Be(c) + Cl_2(g) = BeCl_2(\beta,\alpha,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	14.931	18.120	18.120	0	-118.500	-107.337	78.679
300	14.967	18.212	18.120	.028	-118.494	-107.269	78.144
400	16.462	22.741	18.726	1.606	-118.182	-103.572	56.589
500	17.408	26.524	19.920	3.302	-117.840	-99.962	43.693
600	18.035	29.757	21.295	5.077	-117.479	-96.415	35.119
676*	18.348	31.927	22.371	6.460	-117.197	-93.769	30.315
676	19.557	34.131	22.371	7.950	-115.707	-93.769	30.315
688	19.658	34.476	22.579	8.185	-115.648	-93.380	29.663
688	29.100	37.456	22.579	10.235	-113.598	-93.380	29.663
700	29.100	37.959	22.839	10.584	-113.425	-93.029	29.045
750	29.100	39.967	23.915	12.039	-112.709	-91.597	26.691

*α-$BeCl_2$ metastable below 676 K.

Phase changes: 676 K, β - α transition point of $BeCl_2$; ΔH° = 1.490 kcal/mol.
688 K, melting point of $BeCl_2$; ΔH° = 2.050 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-676 K: $Cp^\circ = 16.361 + 3.844\times10^{-3}T - 2.289\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 16.361\times10^{-3}T + 1.922\times10^{-6}T^2 + 2.289\times10^{2}T^{-1} - 5.817$

676-688 K: $Cp^\circ = 16.591 + 4.388\times10^{-3}T$

$H^\circ - H^\circ_{298} = 16.591\times10^{-3}T + 2.194\times10^{-6}T^2 - 4.268$

688-750 K: $Cp^\circ = 29.100$

$H^\circ - H^\circ_{298} = 29.100\times10^{-3}T - 9.786$

Formation equations (kcal/mol):

298.15-676 K: $\Delta Hf^\circ = -119.536 + 2.793\times10^{-3}T + 0.872\times10^{-6}T^2 + 37.500T^{-1}$

$\Delta Gf^\circ = -119.536 - 2.793\times10^{-3}T\ln T - 0.872\times10^{-6}T^2 + 18.750T^{-1} + 56.877\times10^{-3}T$

676-688 K: $\Delta Hf^\circ = -117.987 + 3.023\times10^{-3}T + 1.144\times10^{-6}T^2 - 191.400T^{-1}$

$\Delta Gf^\circ = -117.987 - 3.023\times10^{-3}T\ln T - 1.144\times10^{-6}T^2 - 95.700T^{-1} + 56.519\times10^{-3}T$

688-750 K: $\Delta Hf^\circ = -123.505 + 15.532\times10^{-3}T - 1.050\times10^{-6}T^2 - 191.400T^{-1}$

$\Delta Gf^\circ = -123.505 - 15.532\times10^{-3}T\ln T + 1.050\times10^{-6}T^2 - 95.700T^{-1} + 144.761\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (187). Other data based on McDonald (157).

$BeCl_2(\alpha,l)$
Beryllium Dichloride
[Formation: $Be(c) + Cl_2(g) = BeCl_2(\alpha,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	15.500	19.760	19.760	0	-117.200	-106.526	78.085
300	15.532	19.856	19.760	.029	-117.193	-106.461	77.556
400	16.911	24.526	20.389	1.655	-116.833	-102.937	56.242
500	17.954	28.415	21.615	3.400	-116.442	-99.510	43.495
600	18.862	31.770	23.033	5.242	-116.014	-96.158	35.025
688	19.608	34.401	24.321	6.935	-115.598	-93.278	29.630
688	29.100	37.381	24.321	8.985	-113.548	-93.278	29.630
700	29.100	37.885	24.551	9.334	-113.375	-92.927	29.013
750	29.100	39.892	25.507	10.789	-112.659	-91.491	26.660

*α-$BeCl_2$ metastable below 676 K.

Phase change: 688 K, melting point of $BeCl_2$; $\Delta H° = 2.050$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-688 K: $Cp° = 14.650 + 7.614\times10^{-3}T - 1.263\times10^{5}T^{-2}$

$H°- H°_{298} = 14.650\times10^{-3}T + 3.807\times10^{-6}T^2 + 1.263\times10^{2}T^{-1} - 5.130$

688-750 K: $Cp° = 29.100$

$H°- H°_{298} = 29.100\times10^{-3}T - 11.036$

Formation equations (kcal/mol):

298.15-688 K: $\Delta Hf° = -117.549 + 1.082\times10^{-3}T + 2.757\times10^{-6}T^2 - 65.100T^{-1}$

$\Delta Gf° = -117.549 - 1.082\times10^{-3}T\ln T - 2.757\times10^{-6}T^2 - 32.550T^{-1} + 44.325\times10^{-3}T$

688-750 K: $\Delta Hf° = -123.455 + 15.532\times10^{-3}T - 1.050\times10^{-6}T^2 - 191.400T^{-1}$

$\Delta Gf° = -123.455 - 15.532\times10^{-3}T\ln T + 1.050\times10^{-6}T^2 - 95.700T^{-1} + 144.836\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (187). Other data based on McDonald (157).

$BeCl_2(g)$

Beryllium Dichloride (ideal gas)

[Formation: $Be(c,l) + Cl_2(g) = BeCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	12.338	60.260	60.260	0	-86.100	-87.501	64.139
300	12.353	60.337	60.260	.023	-86.099	-87.511	63.751
400	13.025	63.988	60.753	1.294	-86.094	-87.983	48.071
500	13.493	66.948	61.706	2.621	-86.121	-88.455	38.663
600	13.822	69.439	62.792	3.988	-86.168	-88.914	32.386
700	14.056	71.589	63.900	5.382	-86.227	-89.372	27.903
800	14.225	73.477	64.981	6.797	-86.296	-89.815	24.536
900	14.351	75.160	66.020	8.226	-86.374	-90.247	21.915
1000	14.446	76.677	67.011	9.666	-86.466	-90.675	19.817
1100	14.519	78.058	67.954	11.114	-86.577	-91.092	18.098
1200	14.576	79.324	68.850	12.569	-86.705	-91.503	16.665
1300	14.621	80.492	69.700	14.029	-86.853	-91.889	15.448
1400	14.658	81.577	70.511	15.493	-87.021	-92.270	14.404
1500	14.689	82.589	71.282	16.961	-87.208	-92.647	13.498
1527	14.696	82.851	71.484	17.358	-87.262	-92.739	13.273
1527	14.696	82.851	71.484	17.358	-87.873	-92.739	13.273
1560	14.704	83.166	71.728	17.843	-87.942	-92.852	13.008
1560	14.704	83.166	71.728	17.843	-90.861	-92.852	13.008
1600	14.714	83.538	72.019	18.431	-90.918	-92.900	12.689
1700	14.735	84.431	72.723	19.903	-91.059	-93.031	11.960
1800	14.752	85.274	73.397	21.378	-91.199	-93.148	11.310
1900	14.768	86.072	74.044	22.854	-91.339	-93.233	10.724
2000	14.781	86.829	74.664	24.331	-91.481	-93.331	10.199

Phase changes: 1527 K, α - β transition point of Be; $\Delta H°$ = 0.611 kcal/mol.
1560 K, melting point of Be; $\Delta H°$ = 2.919 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.878 + 0.600\times10^{-3}T - 1.528\times10^{5}T^{-2}$

$H°- H°_{298} = 13.878\times10^{-3}T + 0.300\times10^{-6}T^2 + 1.528\times10^{2}T^{-1} - 4.677$

Formation equations (kcal/mol):

298.15-1527 K: $\Delta Hf° = -85.996 + 0.310\times10^{-3}T - 0.750\times10^{-6}T^2 - 38.600T^{-1}$

$\Delta Gf° = -85.996 - 0.310\times10^{-3}T\ln T + 0.750\times10^{-6}T^2 - 19.300T^{-1} - 3.288\times10^{-3}T$

1527-1560 K: $\Delta Hf° = -84.413 - 2.649\times10^{-3}T + 0.212\times10^{-6}T^2 + 84.500T^{-1}$

$\Delta Gf° = -84.413 + 2.649\times10^{-3}T\ln T - 0.212\times10^{-6}T^2 + 42.250T^{-1} - 24.575\times10^{-3}T$

1560-2000 K: $\Delta Hf° = -88.361 - 1.989\times10^{-3}T + 0.212\times10^{-6}T^2 + 84.500T^{-1}$

$\Delta Gf° = -88.361 + 1.989\times10^{-3}T\ln T - 0.212\times10^{-6}T^2 + 42.250T^{-1} - 17.191\times10^{-3}T$

Source: Data from JANAF (60).

$(BeCl_2)_2(g)$

Dimeric Beryllium Dichloride (ideal gas)

[Formation: $2Be(c,l) + 2Cl_2(g) = (BeCl_2)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	27.574	91.150	91.150	0	-202.000	-196.046	143.704
300	27.610	91.321	91.151	.051	-201.993	-196.011	142.792
400	29.054	99.481	92.254	2.891	-201.685	-194.065	106.031
500	29.890	106.062	94.378	5.842	-201.442	-192.194	84.007
600	30.406	111.561	96.796	8.859	-201.253	-190.354	69.336
700	30.743	116.275	99.251	11.917	-201.101	-188.559	58.870
800	30.973	120.396	101.641	15.004	-200.982	-186.774	51.024
900	31.136	124.054	103.932	18.110	-200.890	-184.996	44.923
1000	31.256	127.342	106.112	21.230	-200.834	-183.240	40.047
1100	31.346	130.325	108.180	24.360	-200.822	-181.483	36.057
1200	31.416	133.056	110.141	27.498	-200.850	-179.735	32.734
1300	31.471	135.572	112.000	30.643	-200.921	-177.958	29.917
1400	31.514	137.906	113.769	33.792	-201.036	-176.186	27.504
1500	31.550	140.082	115.452	36.945	-201.193	-174.427	25.414
1527	31.558	140.645	115.892	37.797	-201.243	-173.933	24.894
1527	31.558	140.645	115.892	37.797	-202.465	-173.933	24.894
1560	31.567	141.320	116.423	38.839	-202.530	-173.332	24.283
1560	31.567	141.320	116.423	38.839	-208.368	-173.332	24.283
1600	31.579	142.119	117.055	40.102	-208.396	-172.430	23.552
1700	31.604	144.034	118.586	43.261	-208.463	-170.199	21.880
1800	31.624	145.841	120.051	46.422	-208.532	-167.958	20.393
1900	31.642	147.552	121.454	49.586	-208.600	-165.664	19.055
2000	31.656	149.175	122.800	52.751	-208.673	-163.407	17.856

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1527 K, α - β transition point of Be; ΔH° = 0.611 kcal/mol.
1560 K, melting point of Be; ΔH° = 2.919 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 30.947 + 0.522\times10^{-3}T - 3.136\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 30.947\times10^{-3}T + 0.261\times10^{-6}T^2 + 3.136\times10^{2}T^{-1} - 10.302$

Formation equations (kcal/mol):

298.15-1527 K: $\Delta Hf^\circ = -202.741 + 3.811\times10^{-3}T - 1.839\times10^{-6}T^2 - 69.200T^{-1}$

$\Delta Gf^\circ = -202.741 - 3.811\times10^{-3}T\ln T + 1.839\times10^{-6}T^2 - 34.600T^{-1} + 44.009\times10^{-3}T$

1527-1560 K: $\Delta Hf^\circ = -199.573 - 2.107\times10^{-3}T + 0.085\times10^{-6}T^2 + 177.000T^{-1}$

$\Delta Gf^\circ = -199.573 + 2.107\times10^{-3}T\ln T - 0.085\times10^{-6}T^2 + 88.500T^{-1} + 1.434\times10^{-3}T$

1560-2000 K: $\Delta Hf^\circ = -207.471 - 0.787\times10^{-3}T + 0.085\times10^{-6}T^2 + 177.000T^{-1}$

$\Delta Gf^\circ = -207.471 + 0.787\times10^{-3}T\ln T - 0.085\times10^{-6}T^2 + 88.500T^{-1} + 16.202\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (187). Other data from JANAF (60) who estimated molecular constants.

BeF(g)

Beryllium Monofluoride (ideal gas)

[Formation: $Be(c,l) + 0.5F_2(g) = BeF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.140	49.149	49.149	0	-40.600	-47.355	34.712
300	7.144	49.193	49.150	.013	-40.601	-47.399	34.529
400	7.431	51.286	49.433	.741	-40.693	-49.652	27.128
500	7.726	52.977	49.977	1.500	-40.837	-51.878	22.675
600	7.978	54.408	50.600	2.285	-41.012	-54.066	19.693
700	8.178	55.654	51.235	3.093	-41.203	-56.231	17.556
800	8.335	56.756	51.857	3.919	-41.407	-58.363	15.944
900	8.458	57.745	52.457	4.759	-41.619	-60.465	14.683
1000	8.555	58.642	53.032	5.610	-41.846	-62.550	13.670
1100	8.634	59.461	53.579	6.470	-42.091	-64.609	12.836
1200	8.698	60.215	54.102	7.336	-42.354	-66.651	12.139
1300	8.752	60.913	54.598	8.209	-42.634	-68.656	11.542
1400	8.797	61.564	55.074	9.086	-42.935	-70.648	11.029
1500	8.836	62.172	55.527	9.968	-43.253	-72.626	10.581
1527	8.845	62.330	55.646	10.207	-43.343	-73.148	10.469
1527	8.845	62.330	55.646	10.207	-43.954	-73.148	10.469
1560	8.856	62.519	55.789	10.499	-44.066	-73.785	10.337
1560	8.856	62.519	55.789	10.499	-46.985	-73.785	10.337
1600	8.869	62.743	55.960	10.853	-47.094	-74.470	10.172
1700	8.899	63.282	56.375	11.742	-47.362	-76.183	9.794
1800	8.925	63.791	56.773	12.633	-47.632	-77.875	9.455
1900	8.949	64.274	57.155	13.527	-47.898	-79.529	9.148
2000	8.970	64.734	57.523	14.423	-48.165	-81.191	8.872

Phase changes: 1527 K, α - β transition point of Be; $\Delta H° = 0.611$ kcal/mol.
1560 K, melting point of Be; $\Delta H° = 2.919$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.767 + 0.738\times10^{-3}T - 0.753\times10^{5}T^{-2}$

$H°- H°_{298} = 7.767\times10^{-3}T + 0.369\times10^{-6}T^{2} + 0.753\times10^{2}T^{-1} - 2.601$

Formation equations (kcal/mol):

298.15-1527 K: $\Delta Hf° = -39.845 - 1.228\times10^{-3}T - 0.680\times10^{-6}T^{2} - 98.050T^{-1}$

$\Delta Gf° = -39.845 + 1.228\times10^{-3}T\ln T + 0.680\times10^{-6}T^{2} - 49.025T^{-1} - 31.839\times10^{-3}T$

1527-1560 K: $\Delta Hf° = -38.261 - 4.187\times10^{-3}T + 0.282\times10^{-6}T^{2} + 25.050T^{-1}$

$\Delta Gf° = -38.261 + 4.187\times10^{-3}T\ln T - 0.282\times10^{-6}T^{2} + 12.525T^{-1} - 53.126\times10^{-3}T$

1560-2000 K: $\Delta Hf° = -42.210 - 3.527\times10^{-3}T + 0.282\times10^{-6}T^{2} + 25.050T^{-1}$

$\Delta Gf° = -42.210 + 3.527\times10^{-3}T\ln T - 0.282\times10^{-6}T^{2} + 12.525T^{-1} - 45.743\times10^{-3}T$

Source: Data from Chase (25).

BeF_2(c,l)

Beryllium Difluoride

[Formation: $Be(c) + F_2(g) = BeF_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.390	12.750	12.750	0	-245.400	-234.081	171.584
300	12.439	12.827	12.750	.023	-245.398	-234.012	170.476
400	14.985	16.746	13.266	1.392	-245.234	-230.236	125.794
500	17.580	20.369	14.329	3.020	-244.911	-226.524	99.012
500	15.323	20.519	14.329	3.095	-244.836	-226.524	99.012
600	15.948	23.365	15.603	4.657	-244.649	-222.875	81.181
700	16.766	25.883	16.896	6.291	-244.438	-219.267	68.457
800	17.777	28.185	18.164	8.017	-244.172	-215.686	58.922
825	18.060	28.737	18.477	8.465	-244.094	-214.798	56.901
825	20.300	30.095	18.477	9.585	-242.974	-214.798	56.901
900	20.300	31.861	19.520	11.107	-242.570	-212.251	51.541
1000	20.300	34.000	20.863	13.137	-242.058	-208.913	45.657
1100	20.300	35.935	22.147	15.167	-241.576	-205.623	40.853
1200	20.300	37.701	23.370	17.197	-241.120	-202.379	36.858

Phase changes: 500 K, α - β transition point of BeF_2; ΔH° = 0.075 kcal/mol.
825 K, melting point of BeF_2; ΔH° = 1.120 kcal/mol. On cooling, liquid solidifies to vitreous form.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-500 K: $Cp^\circ = 3.913 + 27.086\times10^{-3}T + 0.357\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 3.913\times10^{-3}T + 13.543\times10^{-6}T^2 - 0.357\times10^{2}T^{-1} - 2.251$

500-825 K: $Cp^\circ = 7.465 + 11.950\times10^{-3}T + 4.707\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 7.465\times10^{-3}T + 5.975\times10^{-6}T^2 - 4.707\times10^{2}T^{-1} - 1.190$

825-1200 K: $Cp^\circ = 20.300$

$H^\circ - H^\circ_{298} = 20.300\times10^{-3}T - 7.163$

Formation equations (kcal/mol):

298.15-500 K: $\Delta Hf^\circ = -242.850 - 9.336\times10^{-3}T + 12.407\times10^{-6}T^2 - 259.300T^{-1}$

$\Delta Gf^\circ = -242.850 + 9.336\times10^{-3}T\ln T - 12.407\times10^{-6}T^2 - 129.650T^{-1} - 18.626\times10^{-3}T$

500-825 K: $\Delta Hf^\circ = -241.789 - 5.784\times10^{-3}T + 4.839\times10^{-6}T^2 - 694.300T^{-1}$

$\Delta Gf^\circ = -241.789 + 5.784\times10^{-3}T\ln T - 4.839\times10^{-6}T^2 - 347.150T^{-1} - 1.588\times10^{-3}T$

825-1200 K: $\Delta Hf^\circ = -247.761 + 7.051\times10^{-3}T - 1.136\times10^{-6}T^2 - 223.600T^{-1}$

$\Delta Gf^\circ = -247.761 - 7.051\times10^{-3}T\ln T + 1.136\times10^{-6}T^2 - 111.800T^{-1} + 86.569\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (185). Low-temperature heat capacities and entropy at 298 K from Taylor (236). High-temperature data based on Tamura (235) and Taylor (236).

BeF_2(vitreous)
Beryllium Difluoride
[Formation: $Be(c) + F_2(g) = BeF_2(vit)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	11.850	14.300	14.300	0	-244.280	-233.423	171.102
300	11.913	14.373	14.300	.022	-244.279	-233.357	169.998
400	14.119	18.147	14.799	1.339	-244.167	-229.730	125.517
500	15.124	21.418	15.804	2.807	-244.004	-226.141	98.845
600	15.650	24.227	16.980	4.348	-243.838	-222.581	81.074

*Entropy and heat capacity at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp^\circ = 17.019 - 0.152\times10^{-3}T - 4.554\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 17.019\times10^{-3}T - 0.076\times10^{-6}T^2 + 4.554\times10^{2}T^{-1} - 6.595$

Formation equations (kcal/mol):

298.15-600 K: $\Delta Hf^\circ = -246.074 + 3.770\times10^{-3}T - 1.212\times10^{-6}T^2 + 231.800T^{-1}$

$\Delta Gf^\circ = -246.074 - 3.770\times10^{-3}T\ln T + 1.212\times10^{-6}T^2 + 115.900T^{-1} + 62.244\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Parker (185) and Taylor (236). High-temperature data based on Tamura (235) and Taylor (236). Entropy and heat capacity at 298 K estimated.

$BeF_2(g)$

Beryllium Difluoride (ideal gas)

[Formation: $Be(c,l) + F_2(g) = BeF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	11.081	54.360	54.360	0	-190.250	-191.337	140.252
300	11.100	54.429	54.360	.021	-190.250	-191.345	139.393
400	11.955	57.747	54.807	1.176	-190.300	-191.703	104.740
500	12.573	60.484	55.676	2.404	-190.377	-192.047	83.943
600	13.038	62.819	56.677	3.685	-190.471	-192.369	70.070
700	13.392	64.857	57.703	5.008	-190.571	-192.682	60.157
800	13.663	66.664	58.713	6.361	-190.678	-192.976	52.718
900	13.873	68.286	59.688	7.738	-190.789	-193.252	46.927
1000	14.036	69.756	60.622	9.134	-190.911	-193.522	42.294
1100	14.166	71.100	61.515	10.544	-191.049	-193.777	38.499
1200	14.269	72.337	62.365	11.966	-191.201	-194.023	35.336
1300	14.353	73.483	63.177	13.398	-191.370	-194.244	32.655
1400	14.422	74.549	63.951	14.837	-191.559	-194.458	30.356
1500	14.479	75.546	64.691	16.282	-191.766	-194.669	28.363
1527	14.492	75.804	64.886	16.673	-191.825	-194.714	27.868
1527	14.492	75.804	64.886	16.673	-192.436	-194.714	27.868
1560	14.508	76.114	65.120	17.151	-192.511	-194.771	27.286
1560	14.508	76.114	65.120	17.151	-195.430	-194.771	27.286
1600	14.527	76.482	65.400	17.732	-195.494	-194.752	26.601
1700	14.567	77.364	66.078	19.187	-195.651	-194.711	25.031
1800	14.602	78.198	66.729	20.645	-195.809	-194.657	23.634
1900	14.631	78.988	67.353	22.107	-195.964	-194.569	22.380
2000	14.656	79.739	67.953	23.571	-196.121	-194.495	21.253

Phase changes: 1527 K, α - β transition point of Be; $\Delta H° = 0.611$ kcal/mol.
1560 K, melting point of Be; $\Delta H° = 2.919$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.999 + 1.048\times10^{-3}T - 1.983\times10^{5}T^{-2}$

$H°- H°_{298} = 12.999\times10^{-3}T + 0.524\times10^{-6}T^2 + 1.983\times10^{2}T^{-1} - 4.587$

Formation equations (kcal/mol):

298.15-1527 K: $\Delta Hf° = -190.036 - 0.250\times10^{-3}T - 0.612\times10^{-6}T^2 - 25.300T^{-1}$

$\Delta Gf° = -190.036 + 0.250\times10^{-3}T\ln T + 0.612\times10^{-6}T^2 - 12.650T^{-1} - 5.829\times10^{-3}T$

1527-1560 K: $\Delta Hf° = -188.453 - 3.209\times10^{-3}T + 0.350\times10^{-6}T^2 + 97.800T^{-1}$

$\Delta Gf° = -188.453 + 3.209\times10^{-3}T\ln T - 0.350\times10^{-6}T^2 + 48.900T^{-1} - 27.116\times10^{-3}T$

1560-2000 K: $\Delta Hf° = -192.401 - 2.549\times10^{-3}T + 0.350\times10^{-6}T^2 + 97.800T^{-1}$

$\Delta Gf° = -192.401 + 2.549\times10^{-3}T\ln T - 0.350\times10^{-6}T^2 + 48.900T^{-1} - 19.732\times10^{-3}T$

Source: Data from JANAF (60).

BeI(g)

Beryllium Monoiodide (ideal gas)

[Formation: $Be(c,l) + 0.5I_2(c,l,g) = BeI(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.001	56.688	56.688	0	40.600	28.513	-20.901
300	8.009	56.738	56.688	.015	40.596	28.437	-20.716
386.8	8.308	58.813	56.942	.724	40.327	24.952	-14.098
386.8	8.308	58.813	56.942	.724	38.472	24.952	-14.098
400	8.353	59.093	57.008	.834	38.393	24.492	-13.382
458.4	8.474	60.241	57.347	1.327	38.036	22.486	-10.721
458.4	8.474	60.241	57.347	1.327	33.026	22.486	-10.721
500	8.561	60.981	57.619	1.681	32.980	21.533	-9.412
600	8.694	62.555	58.315	2.544	32.849	19.259	-7.015
700	8.785	63.902	59.019	3.418	32.699	17.001	-5.308
800	8.850	65.080	59.705	4.300	32.532	14.771	-4.035
900	8.900	66.125	60.361	5.188	32.351	12.565	-3.051
1000	8.939	67.065	60.985	6.080	32.153	10.375	-2.268
1100	8.972	67.918	61.577	6.975	31.932	8.207	-1.631
1200	9.000	68.700	62.138	7.874	31.694	6.056	-1.103
1300	9.024	69.422	62.672	8.775	31.434	3.936	-.662
1400	9.046	70.091	63.177	9.679	31.154	1.833	-.286
1500	9.066	70.716	63.660	10.584	30.854	-.263	.038
1527	9.071	70.878	63.786	10.829	30.769	-.816	.117
1527	9.071	70.878	63.786	10.829	30.158	-.816	.117
1560	9.077	71.072	63.938	11.129	30.054	-1.492	.209
1560	9.077	71.072	63.938	11.129	27.135	-1.492	.209
1600	9.085	71.302	64.119	11.492	27.033	-2.223	.304
1700	9.103	71.853	64.558	12.401	26.780	-4.055	.521
1800	9.119	72.374	64.978	13.312	26.528	-5.867	.712
1900	9.135	72.867	65.380	14.225	26.278	-7.641	.879
2000	9.151	73.336	65.767	15.139	26.028	-9.422	1.030

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
1527 K, α - β transition point of Be; $\Delta H°$ = 0.611 kcal/mol.
1560 K, melting point of Be; $\Delta H°$ = 2.919 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.729 + 0.252\times10^{-3}T - 0.714\times10^{5}T^{-2}$

$H°- H°_{298} = 8.729\times10^{-3}T + 0.126\times10^{-6}T^{2} + 0.714\times10^{2}T^{-1} - 2.853$

BeI(g) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = 41.645 - 2.451\times10^{-3}T - 1.582\times10^{-6}T^2 - 51.700T^{-1}$

$\Delta Gf^\circ = 41.645 + 2.451\times10^{-3}T\ln T + 1.582\times10^{-6}T^2 - 25.850T^{-1} - 58.186\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = 40.917 - 5.653\times10^{-3}T - 0.836\times10^{-6}T^2 - 51.700T^{-1}$

$\Delta Gf^\circ = 40.917 + 5.653\times10^{-3}T\ln T + 0.836\times10^{-6}T^2 - 25.850T^{-1} - 75.093\times10^{-3}T$

458.4-1527 K: $\Delta Hf^\circ = 33.560 - 0.483\times10^{-3}T - 0.870\times10^{-6}T^2 - 59.350T^{-1}$

$\Delta Gf^\circ = 33.560 + 0.483\times10^{-3}T\ln T + 0.870\times10^{-6}T^2 - 29.675T^{-1} - 27.362\times10^{-3}T$

1527-1560 K: $\Delta Hf^\circ = 35.144 - 3.442\times10^{-3}T + 0.092\times10^{-6}T^2 + 63.750T^{-1}$

$\Delta Gf^\circ = 35.144 + 3.442\times10^{-3}T\ln T - 0.092\times10^{-6}T^2 + 31.875T^{-1} - 48.649\times10^{-3}T$

1560-2000 K: $\Delta Hf^\circ = 31.196 - 2.782\times10^{-3}T + 0.092\times10^{-6}T^2 + 63.750T^{-1}$

$\Delta Gf^\circ = 31.196 + 2.782\times10^{-3}T\ln T - 0.092\times10^{-6}T^2 + 31.875T^{-1} - 41.265\times10^{-3}T$

Source: Data from Chase (26).

BeI_2(c,l,g)

Beryllium Diiodide

[Formation: $Be(c,l) + I_2(c,l,g) = BeI_2(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	16.482	28.800	28.800	0	-45.100	-44.734	32.790
300	16.522	28.902	28.800	.031	-45.100	-44.732	32.587
386.8	18.128	33.314	29.332	1.540	-45.173	-44.618	25.210
386.8	18.128	33.314	29.332	1.540	-48.882	-44.618	25.210
400	18.372	33.926	29.473	1.781	-48.958	-44.472	24.298
458.4	19.038	36.483	30.204	2.878	-49.273	-43.794	20.879
458.4	19.038	36.483	30.204	2.878	-59.294	-43.794	20.879
500	19.512	38.157	30.797	3.680	-59.078	-42.395	18.531
600	20.122	41.773	32.333	5.664	-58.536	-39.106	14.244
700	20.427	44.899	33.910	7.692	-57.982	-35.915	11.213
753	20.541	46.395	34.738	8.778	-57.687	-34.254	9.942
753	27.000	53.035	34.738	13.778	-52.687	-34.254	9.942
759.4	27.000	53.264	34.893	13.951	-52.611	-34.097	9.813
759.4	14.451	82.629	34.893	36.251	-30.311	-34.097	9.813
800	14.495	83.384	37.335	36.839	-30.334	-34.300	9.370
900	14.574	85.096	42.549	38.292	-30.402	-34.789	8.448
1000	14.632	86.634	46.881	39.753	-30.484	-35.273	7.709
1100	14.677	88.031	50.560	41.218	-30.588	-35.749	7.103
1200	14.711	89.310	53.737	42.688	-30.710	-36.218	6.596
1300	14.739	90.488	56.519	44.160	-30.853	-36.664	6.164
1400	14.760	91.581	58.985	45.635	-31.018	-37.104	5.792
1500	14.778	92.600	61.192	47.112	-31.203	-37.543	5.470
1527	14.782	92.864	61.750	47.511	-31.257	-37.651	5.389
1527	14.782	92.864	61.750	47.511	-31.868	-37.651	5.389
1560	14.787	93.181	62.412	47.999	-31.935	-37.783	5.293
1560	14.787	93.181	62.412	47.999	-34.854	-37.783	5.293
1600	14.793	93.555	63.186	48.591	-34.910	-37.856	5.171
1700	14.805	94.452	64.998	50.071	-35.050	-38.047	4.891
1800	14.816	95.298	66.658	51.552	-35.190	-38.223	4.641
1900	14.825	96.100	68.187	53.034	-35.331	-38.371	4.414
2000	14.832	96.860	69.602	54.517	-35.472	-38.528	4.210

*Data estimated except temperature of fusion.

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
753 K, melting point of BeI_2; $\Delta H°$ = 5.000 kcal/mol.
759.4 K, boiling point of BeI_2 to monomer; $\Delta H°$ = 22.300 kcal/mol.
1527 K, α - β transition point of Be; $\Delta H°$ = 0.611 kcal/mol.
1560 K, melting point of Be; $\Delta H°$ = 2.919 kcal/mol.

BeI_2(c,l,g) - Continued

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-753 K: $Cp^\circ = 19.387 + 2.606\times10^{-3}T - 3.273\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.387\times10^{-3}T + 1.303\times10^{-6}T^2 + 3.273\times10^{2}T^{-1} - 6.994$

753-759.4 K: $Cp^\circ = 27.000$

$H^\circ - H^\circ_{298} = 27.000\times10^{-3}T - 6.553$

759.4-2000 K: $Cp^\circ = 14.871 + 0.010\times10^{-3}T - 2.469\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.871\times10^{-3}T + 0.005\times10^{-6}T^2 + 2.469\times10^{2}T^{-1} + 24.630$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -46.210 + 1.769\times10^{-3}T - 1.151\times10^{-6}T^2 + 204.200T^{-1}$

$\Delta Gf^\circ = -46.210 - 1.769\times10^{-3}T\ln T + 1.151\times10^{-6}T^2 + 102.100T^{-1} + 13.538\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -47.665 - 4.635\times10^{-3}T + 0.341\times10^{-6}T^2 + 204.200T^{-1}$

$\Delta Gf^\circ = -47.665 + 4.635\times10^{-3}T\ln T - 0.341\times10^{-6}T^2 + 102.100T^{-1} - 20.277\times10^{-3}T$

458.4-753 K: $\Delta Hf^\circ = -62.378 + 5.705\times10^{-3}T + 0.273\times10^{-6}T^2 + 188.900T^{-1}$

$\Delta Gf^\circ = -62.378 - 5.705\times10^{-3}T\ln T - 0.273\times10^{-6}T^2 + 94.450T^{-1} + 75.186\times10^{-3}T$

753-759.4 K: $\Delta Hf^\circ = -61.937 + 13.318\times10^{-3}T - 1.030\times10^{-6}T^2 - 138.400T^{-1}$

$\Delta Gf^\circ = -61.937 - 13.318\times10^{-3}T\ln T + 1.030\times10^{-6}T^2 - 69.200T^{-1} + 124.337\times10^{-3}T$

759.4-1527 K: $\Delta Hf^\circ = -30.755 + 1.189\times10^{-3}T - 1.025\times10^{-6}T^2 + 108.500T^{-1}$

$\Delta Gf^\circ = -30.755 - 1.189\times10^{-3}T\ln T + 1.025\times10^{-6}T^2 + 54.250T^{-1} + 2.618\times10^{-3}T$

1527-1560 K: $\Delta Hf^\circ = -29.171 - 1.770\times10^{-3}T - 0.063\times10^{-6}T^2 + 231.600T^{-1}$

$\Delta Gf^\circ = -29.171 + 1.770\times10^{-3}T\ln T + 0.063\times10^{-6}T^2 + 115.800T^{-1} - 18.669\times10^{-3}T$

1560-2000 K: $\Delta Hf^\circ = -33.120 - 1.110\times10^{-3}T - 0.063\times10^{-6}T^2 + 231.600T^{-1}$

$\Delta Gf^\circ = -33.120 + 1.110\times10^{-3}T\ln T + 0.063\times10^{-6}T^2 + 115.800T^{-1} - 11.285\times10^{-3}T$

Source: Data from Chase (26) who estimated all except temperature of fusion.

$BeI_2(g)$

Beryllium Diiodide (ideal gas)

[Formation: $Be(c,l) + I_2(c,l,g) = BeI_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	13.131	69.649	69.649	0	-15.300	-27.113	19.874
300	13.142	69.730	69.650	.024	-15.307	-27.187	19.806
386.8	13.592	73.130	70.063	1.186	-15.727	-30.573	17.274
386.8	13.592	73.130	70.063	1.186	-19.436	-30.573	17.274
400	13.660	73.587	70.172	1.366	-19.573	-30.951	16.911
458.4	13.860	75.464	70.727	2.171	-20.179	-32.569	15.528
458.4	13.860	75.464	70.727	2.171	-30.200	-32.569	15.528
500	14.003	76.674	71.172	2.751	-30.207	-32.783	14.329
600	14.231	79.249	72.311	4.163	-30.237	-33.292	12.127
700	14.386	81.455	73.464	5.594	-30.280	-33.802	10.553
800	14.495	83.384	74.585	7.039	-30.334	-34.300	9.370
900	14.574	85.096	75.660	8.492	-30.402	-34.790	8.448
1000	14.632	86.634	76.681	9.953	-30.484	-35.273	7.709
1100	14.677	88.031	77.651	11.418	-30.588	-35.749	7.103
1200	14.711	89.310	78.570	12.888	-30.710	-36.218	6.596
1300	14.739	90.488	79.442	14.360	-30.853	-36.664	6.164
1400	14.760	91.581	80.270	15.835	-31.018	-37.104	5.792
1500	14.778	92.600	81.059	17.312	-31.203	-37.543	5.470
1527	14.782	92.864	81.265	17.711	-31.257	-37.651	5.389
1527	14.782	92.864	81.265	17.711	-31.868	-37.651	5.389
1560	14.787	93.181	81.514	18.199	-31.935	-37.783	5.293
1560	14.787	93.181	81.514	18.199	-34.854	-37.783	5.293
1600	14.793	93.555	81.811	18.791	-34.910	-37.856	5.171
1700	14.805	94.452	82.528	20.271	-35.050	-38.047	4.891
1800	14.816	95.298	83.214	21.752	-35.190	-38.223	4.641
1900	14.825	96.100	83.872	23.234	-35.331	-38.371	4.414
2000	14.832	96.860	84.502	24.717	-35.472	-38.528	4.210

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
1527 K, α - β transition point of Be; ΔH° = 0.611 kcal/mol.
1560 K, melting point of Be; ΔH° = 2.919 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 14.287 + 0.388\times10^{-3}T - 1.130\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.287\times10^{-3}T + 0.194\times10^{-6}T^2 + 1.130\times10^{2}T^{-1} - 4.656$

$BeI_2(g)$ - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -14.072 - 3.331\times10^{-3}T - 2.260\times10^{-6}T^2 - 10.100T^{-1}$

$\Delta Gf^\circ = -14.072 + 3.331\times10^{-3}T\ln T + 2.260\times10^{-6}T^2 - 5.050T^{-1} - 63.335\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -15.527 - 9.735\times10^{-3}T - 0.768\times10^{-6}T^2 - 10.100T^{-1}$

$\Delta Gf^\circ = -15.527 + 9.735\times10^{-3}T\ln T + 0.768\times10^{-6}T^2 - 5.050T^{-1} - 97.150\times10^{-3}T$

458.4-1527 K: $\Delta Hf^\circ = -30.240 + 0.605\times10^{-3}T - 0.836\times10^{-6}T^2 - 25.400T^{-1}$

$\Delta Gf^\circ = -30.240 - 0.605\times10^{-3}T\ln T + 0.836\times10^{-6}T^2 - 12.700T^{-1} - 1.688\times10^{-3}T$

1527-1560 K: $\Delta Hf^\circ = -28.657 - 2.354\times10^{-3}T + 0.126\times10^{-6}T^2 + 97.700T^{-1}$

$\Delta Gf^\circ = -28.657 + 2.354\times10^{-3}T\ln T - 0.126\times10^{-6}T^2 + 48.850T^{-1} - 22.975\times10^{-3}T$

1560-2000 K: $\Delta Hf^\circ = -32.605 - 1.694\times10^{-3}T + 0.126\times10^{-6}T^2 + 97.700T^{-1}$

$\Delta Gf^\circ = -32.605 + 1.694\times10^{-3}T\ln T - 0.126\times10^{-6}T^2 + 48.850T^{-1} - 15.591\times10^{-3}T$

Source: Data from Chase (26) who estimated some molecular constants.

$BiBr_3(c,l)$

Bismuth Tribromide

[Formation: $Bi(c,l) + 1.5Br_2(l,g) = BiBr_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	24.100	46.700	46.700	0	-66.000	-59.611	43.696
300	24.120	46.849	46.700	.045	-66.016	-59.569	43.396
332.6	24.560	49.360	46.839	.838	-66.304	-58.854	38.672
332.6	24.560	49.360	46.839	.838	-76.902	-58.854	38.672
400	25.470	53.973	47.663	2.524	-76.521	-55.240	30.181
431	25.880	55.889	48.186	3.320	-76.332	-53.597	27.177
431	21.000	57.734	48.186	4.115	-75.537	-53.597	27.177
491.7	21.000	60.501	49.539	5.390	-75.469	-50.511	22.451
491.7	34.560	70.517	49.539	10.315	-70.544	-50.511	22.451
500	34.470	71.096	49.892	10.602	-70.424	-50.174	21.931
544.59	34.002	74.021	51.750	12.129	-69.801	-48.397	19.422
544.59	34.002	74.021	51.750	12.129	-72.501	-48.397	19.422
600	33.420	77.288	53.960	13.997	-71.769	-45.982	16.749
700	32.370	82.362	57.668	17.286	-70.512	-41.785	13.046
800	31.320	86.615	61.026	20.471	-69.348	-37.756	10.314
900	30.270	90.243	64.076	23.550	-68.284	-33.879	8.227
1000	29.210	93.378	66.854	26.524	-67.319	-30.104	6.579

*Heat capacity at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
431 K, α - β transition point of $BiBr_3$; ΔH° = 0.795 kcal/mol.
491.7 K, melting point of $BiBr_3$; ΔH° = 4.925 kcal/mol.
544.59 K, melting point of Bi; ΔH° = 2.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-431 K: $Cp^\circ = 20.089 + 13.446\times10^{-3}T$

$H^\circ - H^\circ_{298} = 20.089\times10^{-3}T + 6.723\times10^{-6}T^2 - 6.587$

431-491.7 K: $Cp^\circ = 21.000$

$H^\circ - H^\circ_{298} = 21.000\times10^{-3}T - 4.936$

491.7-1000 K: $Cp^\circ = 39.738 - 10.524\times10^{-3}T$

$H^\circ - H^\circ_{298} = 39.738\times10^{-3}T - 5.262\times10^{-6}T^2 - 7.952$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -63.493 - 10.370\times10^{-3}T + 3.671\times10^{-6}T^2 + 77.100T^{-1}$

$\Delta Gf^\circ = -63.493 + 10.370\times10^{-3}T\ln T - 3.671\times10^{-6}T^2 + 38.550T^{-1} - 45.406\times10^{-3}T$

332.6-431 K: $\Delta Hf^\circ = -78.494 + 3.371\times10^{-3}T + 3.439\times10^{-6}T^2 + 30.000T^{-1}$

$\Delta Gf^\circ = -78.494 - 3.371\times10^{-3}T\ln T - 3.439\times10^{-6}T^2 + 15.000T^{-1} + 79.626\times10^{-3}T$

431-491.7 K: $\Delta Hf^\circ = -76.842 + 4.282\times10^{-3}T - 3.285\times10^{-6}T^2 + 30.000T^{-1}$

$\Delta Gf^\circ = -76.842 - 4.282\times10^{-3}T\ln T + 3.285\times10^{-6}T^2 + 15.000T^{-1} + 78.424\times10^{-3}T$

491.7-544.59 K: $\Delta Hf^\circ = -79.859 + 23.020\times10^{-3}T - 8.547\times10^{-6}T^2 + 30.000T^{-1}$

$\Delta Gf^\circ = -79.859 - 23.020\times10^{-3}T\ln T + 8.547\times10^{-6}T^2 + 15.000T^{-1} + 198.107\times10^{-3}T$

544.59-1000 K: $\Delta Hf^\circ = -82.635 + 20.490\times10^{-3}T - 5.503\times10^{-6}T^2 + 330.600T^{-1}$

$\Delta Gf^\circ = -82.635 - 20.490\times10^{-3}T\ln T + 5.503\times10^{-6}T^2 + 165.300T^{-1} + 188.417\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Cubicciotti (42). High-temperature data based on Cubicciotti (50). Heat capacity at 298 K estimated.

$BiBr_3(g)$

Bismuth Tribromide (ideal gas)

[Formation: $Bi(c,l) + 1.5Br_2(l,g) = BiBr_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.410	91.850	91.850	0	-37.500	-44.573	32.672
300	19.420	91.980	91.850	.039	-37.521	-44.615	32.501
332.6	19.482	93.987	91.963	.673	-37.970	-45.363	29.807
332.6	19.482	93.987	91.963	.673	-48.567	-45.363	29.807
400	19.610	97.590	92.612	1.991	-48.553	-44.719	24.433
500	19.700	101.940	94.036	3.952	-48.574	-43.746	19.121
544.59	19.722	103.624	94.753	4.831	-48.599	-43.316	17.383
544.59	19.722	103.624	94.753	4.831	-51.299	-43.316	17.383
600	19.750	105.590	95.705	5.931	-51.335	-42.529	15.491
700	19.780	108.620	97.330	7.903	-51.395	-41.049	12.816
800	19.810	111.280	98.916	9.891	-51.428	-39.568	10.809
900	19.820	113.530	100.357	11.856	-51.478	-38.031	9.235
1000	19.830	115.650	101.803	13.847	-51.496	-36.553	7.989
1100	19.830	117.570	103.168	15.842	-51.507	-35.081	6.970
1200	19.840	119.390	104.527	17.835	-51.519	-33.684	6.135
1300	19.840	120.840	105.604	19.807	-51.554	-32.031	5.385
1400	19.850	122.380	106.815	21.791	-51.579	-30.627	4.781
1500	19.850	123.720	107.862	23.787	-51.595	-29.073	4.236

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
544.59 K, melting point of Bi; $\Delta H°$ = 2.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 19.912 - 0.036\times10^{-3}T - 0.437\times10^{5}T^{-2}$

$H°- H°_{298} = 19.912\times10^{-3}T - 0.018\times10^{-6}T^2 + 0.437\times10^{2}T^{-1} - 6.082$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -34.488 - 10.547\times10^{-3}T - 3.070\times10^{-6}T^2 + 120.800T^{-1}$

$\Delta Gf° = -34.488 + 10.547\times10^{-3}T\ln T + 3.070\times10^{-6}T^2 + 60.400T^{-1} - 95.516\times10^{-3}T$

332.6-544.59 K: $\Delta Hf° = -49.488 + 3.194\times10^{-3}T - 3.303\times10^{-6}T^2 + 73.700T^{-1}$

$\Delta Gf° = -49.488 - 3.194\times10^{-3}T\ln T + 3.303\times10^{-6}T^2 + 36.850T^{-1} + 29.517\times10^{-3}T$

544.59-1500 K: $\Delta Hf° = -52.265 + 0.664\times10^{-3}T - 0.260\times10^{-6}T^2 + 374.300T^{-1}$

$\Delta Gf° = -52.265 - 0.664\times10^{-3}T\ln T + 0.260\times10^{-6}T^2 + 187.150T^{-1} + 19.827\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Cubicciotti (42). Other data from Manley (154).

$BiCl_3(c,l)$

Bismuth Trichloride

[Formation: $Bi(c,l) + 1.5Cl_2(g) = BiCl_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	24.000	42.300	42.300	0	-90.600	-75.336	55.222
300	24.025	42.449	42.302	.044	-90.590	-75.241	54.812
400	25.427	49.553	43.261	2.517	-89.982	-70.217	38.364
500	26.826	55.377	45.117	5.130	-89.307	-65.349	28.564
506.7	26.920	55.735	45.255	5.310	-89.260	-65.028	28.048
506.7	34.300	66.905	45.255	10.970	-83.600	-65.028	28.048
544.59	34.300	69.379	46.848	12.270	-83.057	-63.662	25.548
544.59	34.300	69.379	46.848	12.270	-85.757	-63.662	25.548
600	34.300	72.702	49.085	14.170	-84.979	-61.454	22.384
700	34.300	77.989	52.846	17.600	-83.559	-57.644	17.997

*Heat capacity at 298 K estimated.

Phase changes: 506.7 K, melting point of $BiCl_3$; ΔH° = 5.660 kcal/mol.
544.59 K, melting point of Bi; ΔH° = 2.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-506.7 K: $Cp^\circ = 19.832 + 13.990\times10^{-3}T$

$H^\circ - H^\circ_{298} = 19.832\times10^{-3}T + 6.995\times10^{-6}T^2 - 6.535$

506.7-700 K: $Cp^\circ = 34.300$

$H^\circ - H^\circ_{298} = 34.300\times10^{-3}T - 6.410$

Formation equations (kcal/mol):

298.15-506.7 K: $\Delta Hf^\circ = -91.815 + 3.269\times10^{-3}T + 3.661\times10^{-6}T^2 - 25.350T^{-1}$

$\Delta Gf^\circ = -91.815 - 3.269\times10^{-3}T\ln T - 3.661\times10^{-6}T^2 - 12.675T^{-1} + 75.127\times10^{-3}T$

506.7-544.59 K: $\Delta Hf^\circ = -91.690 + 17.736\times10^{-3}T - 3.334\times10^{-6}T^2 - 25.350T^{-1}$

$\Delta Gf^\circ = -91.690 - 17.736\times10^{-3}T\ln T + 3.334\times10^{-6}T^2 - 12.675T^{-1} + 161.441\times10^{-3}T$

544.59-700 K: $\Delta Hf^\circ = -94.467 + 15.206\times10^{-3}T - 0.291\times10^{-6}T^2 + 275.250T^{-1}$

$\Delta Gf^\circ = -94.467 - 15.206\times10^{-3}T\ln T + 0.291\times10^{-6}T^2 + 137.625T^{-1} + 151.751\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (252). High-temperature data based on Topol (242). Heat capacity at 298 K estimated.

$BiCl_3(g)$

Bismuth Trichloride (ideal gas)

[Formation: $Bi(c,l) + 1.5Cl_2(g) = BiCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	19.020	85.400	85.400	0	-63.400	-60.986	44.704
300	19.030	85.520	85.403	.035	-63.399	-60.972	44.417
400	19.390	91.050	86.150	1.960	-63.340	-60.173	32.876
500	19.550	95.390	87.570	3.910	-63.327	-59.375	25.953
544.59	19.590	97.062	88.280	4.783	-63.344	-59.025	23.687
544.59	19.590	97.062	88.280	4.783	-66.044	-59.025	23.687
600	19.640	98.970	89.195	5.865	-66.084	-58.320	21.243
700	19.700	102.000	90.807	7.835	-66.124	-57.017	17.801
800	19.730	104.630	92.374	9.805	-66.160	-55.711	15.219

Phase change: 544.59 K, melting point of Bi; ΔH° = 2.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp^\circ = 19.850 - 0.740\times10^5 T^{-2}$

$H^\circ - H^\circ_{298} = 19.850\times10^{-3} T + 0.740\times10^2 T^{-1} - 6.166$

Formation equations (kcal/mol):

298.15-544.59 K: $\Delta Hf^\circ = -64.247 + 3.287\times10^{-3} T - 3.334\times10^{-6} T^2 + 48.650 T^{-1}$

$\Delta Gf^\circ = -64.247 - 3.287\times10^{-3} T \ln T + 3.334\times10^{-6} T^2 + 24.325 T^{-1} + 28.392\times10^{-3} T$

544.59-800 K: $\Delta Hf^\circ = -67.023 + 0.757\times10^{-3} T - 0.291\times10^{-6} T^2 + 349.250 T^{-1}$

$\Delta Gf^\circ = -67.023 - 0.757\times10^{-3} T \ln T + 0.291\times10^{-6} T^2 + 174.625 T^{-1} + 18.702\times10^{-3} T$

Sources: Enthalpy of formation at 298 K based on Imperatori (104). Entropy at 298 K from Kelley (118). Other data from Kelley (117).

BiF_3(c,l)

Bismuth Trifluoride

[Formation: $Bi(c,l) + 1.5F_2(g) = BiF_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	20.500	29.300	29.300	0	-217.300	-200.328	146.842
300	20.565	29.427	29.300	.038	-217.294	-200.222	145.860
400	23.087	35.723	30.140	2.233	-216.874	-194.591	106.318
500	24.642	41.050	31.804	4.623	-216.348	-189.078	82.645
544.59	25.355	43.186	32.650	5.738	-216.094	-186.659	74.907
544.59	25.355	43.186	32.650	5.738	-218.794	-186.659	74.907
600	26.242	45.677	33.739	7.163	-218.461	-183.408	66.806
700	28.771	49.894	35.748	9.902	-217.687	-177.623	55.456
800	33.062	53.992	37.772	12.976	-216.584	-171.967	46.979
900	39.933	58.254	39.808	16.601	-214.932	-166.485	40.428
922	41.871	59.241	40.261	17.500	-214.468	-165.307	39.184
922	44.100	64.805	40.261	22.630	-209.338	-165.307	39.184
1000	44.100	68.386	42.316	26.070	-207.442	-161.656	35.329
1100	44.100	72.590	44.881	30.480	-205.014	-157.197	31.232

*Heat capacity at 298 K estimated.

Phase changes: 544.59 K, melting point of Bi; $\Delta H° = 2.700$ kcal/mol.
922 K, melting point of BiF_3; $\Delta H° = 5.130$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-922 K: $Cp° = 9.313 + 29.438\times10^{-3}T + 2.140\times10^{5}T^{-2}$

$H°- H°_{298} = 9.313\times10^{-3}T + 14.719\times10^{-6}T^2 - 2.140\times10^{2}T^{-1} - 3.367$

922-1100 K: $Cp° = 44.100$

$H°- H°_{298} = 44.100\times10^{-3}T - 18.030$

Formation equations (kcal/mol):

298.15-544.59 K: $\Delta Hf° = -215.317 - 6.772\times10^{-3}T + 11.256\times10^{-6}T^2 - 287.650T^{-1}$

$\Delta Gf° = -215.317 + 6.772\times10^{-3}T\ln T - 11.256\times10^{-6}T^2 - 143.825T^{-1} + 16.662\times10^{-3}T$

544.59-922 K: $\Delta Hf° = -218.093 - 9.302\times10^{-3}T + 14.299\times10^{-6}T^2 + 12.950T^{-1}$

$\Delta Gf° = -218.093 + 9.302\times10^{-3}T\ln T - 14.299\times10^{-6}T^2 + 6.475T^{-1} + 6.972\times10^{-3}T$

922-1100 K: $\Delta Hf° = -232.757 + 25.485\times10^{-3}T - 0.420\times10^{-6}T^2 + 226.950T^{-1}$

$\Delta Gf° = -232.757 - 25.485\times10^{-3}T\ln T + 0.420\times10^{-6}T^2 + 113.475T^{-1} + 246.654\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Cubicciotti (44) and Wagman (252, 255). Entropy at 298 K and high-temperature data based on Cubicciotti (44). Heat capacity at 298 K estimated.

$BiF_3(g)$

Bismuth Trifluoride (ideal gas)

[Formation: $Bi(c,l) + 1.5F_2(g) = BiF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	17.360	75.920	75.920	0	-169.200	-166.128	121.773
300	17.390	76.030	75.930	.030	-169.202	-166.111	121.010
400	18.440	81.200	76.625	1.830	-169.176	-165.084	90.197
500	18.920	85.370	77.970	3.700	-169.171	-164.061	71.710
544.59	19.045	86.992	78.643	4.546	-169.186	-163.607	65.656
544.59	19.045	86.992	78.643	4.546	-171.886	-163.607	65.656
600	19.200	88.840	79.490	5.610	-171.913	-162.759	59.284
700	19.360	91.820	81.049	7.540	-171.949	-161.233	50.339
800	19.480	94.410	82.560	9.480	-171.980	-159.697	43.627
900	19.560	96.710	84.010	11.430	-172.003	-158.167	38.408
1000	19.620	98.770	85.380	13.390	-172.022	-156.619	34.229

*Data except enthalpy of formation at 298 K estimated.

Phase change: 544.59 K, melting point of Bi; ΔH° = 2.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 19.720 + 0.110\times10^{-3}T - 2.126\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.720\times10^{-3}T + 0.055\times10^{-6}T^2 + 2.126\times10^{2}T^{-1} - 6.597$

Formation equations (kcal/mol):

298.15-544.59 K: $\Delta Hf^\circ = -170.447 + 3.635\times10^{-3}T - 3.408\times10^{-6}T^2 + 138.950T^{-1}$

$\Delta Gf^\circ = -170.447 - 3.635\times10^{-3}T\ln T + 3.408\times10^{-6}T^2 + 69.475T^{-1} + 33.400\times10^{-3}T$

544.59-1000 K: $\Delta Hf^\circ = -173.224 + 1.105\times10^{-3}T - 0.365\times10^{-6}T^2 + 439.550T^{-1}$

$\Delta Gf^\circ = -173.224 - 1.105\times10^{-3}T\ln T + 0.365\times10^{-6}T^2 + 219.775T^{-1} + 23.710\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Cubicciotti (44). Other data based those estimated by Cubicciotti (44).

BiI_3(c,l)

Bismuth Triiodide

[Formation: $Bi(c,l) + 1.5I_2(c,l,g) = BiI_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	25.300	53.700	53.700	0	-36.000	-35.554	26.061
300	25.300	53.860	53.700	.050	-35.997	-35.547	25.896
386.8	24.606	60.126	54.475	2.186	-36.210	-35.403	20.003
386.8	24.606	60.126	54.475	2.186	-41.774	-35.403	20.003
400	24.500	60.950	54.675	2.510	-41.916	-35.183	19.223
458.4	25.084	64.313	55.701	3.948	-42.543	-34.155	16.284
458.4	25.084	64.313	55.701	3.948	-57.575	-34.155	16.284
500	25.500	66.510	56.510	5.000	-57.361	-32.036	14.003
544.59	26.303	68.723	57.421	6.155	-57.116	-29.791	11.955
544.59	26.303	68.723	57.421	6.155	-59.816	-29.791	11.955
600	27.300	71.320	58.587	7.640	-59.475	-26.756	9.746
681.8	29.000	74.910	60.329	9.940	-58.845	-22.332	7.158
681.8	36.000	88.620	60.329	19.290	-49.495	-22.332	7.158
700	36.000	89.570	61.070	19.950	-49.206	-21.605	6.745
800	36.000	94.380	64.942	23.550	-47.635	-17.767	4.854
900	36.000	98.620	68.453	27.150	-46.059	-14.134	3.432
1000	36.000	102.410	71.660	30.750	-44.475	-10.662	2.330

*Heat capacity at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; $\Delta H° = 3.709$ kcal/mol.
458.4 K, boiling point of I_2; $\Delta H° = 10.021$ kcal/mol.
544.59 K, melting point of Bi; $\Delta H° = 2.700$ kcal/mol.
681.8 K, melting point of BiI_3; $\Delta H° = 9.350$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-681.8 K: $Cp° = 9.790 + 25.964\times10^{-3}T + 6.906\times10^{5}T^{-2}$

$H°- H°_{298} = 9.790\times10^{-3}T + 12.982\times10^{-6}T^2 - 6.906\times10^{2}T^{-1} - 1.757$

681.8-1000 K: $Cp° = 36.000$

$H°- H°_{298} = 36.000\times10^{-3}T - 5.255$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -30.782 - 12.849\times10^{-3}T + 7.542\times10^{-6}T^2 - 613.500T^{-1}$

$\Delta Gf° = -30.782 + 12.849\times10^{-3}T\ln T - 7.542\times10^{-6}T^2 - 306.750T^{-1} - 83.511\times10^{-3}T$

386.8-458.4 K: $\Delta Hf° = -32.965 - 22.455\times10^{-3}T + 9.780\times10^{-6}T^2 - 613.500T^{-1}$

$\Delta Gf° = -32.965 + 22.455\times10^{-3}T\ln T - 9.780\times10^{-6}T^2 - 306.750T^{-1} - 134.234\times10^{-3}T$

458.4-544.59 K: $\Delta Hf° = -55.034 - 6.944\times10^{-3}T + 9.678\times10^{-6}T^2 - 636.450T^{-1}$

$\Delta Gf° = -55.034 + 6.944\times10^{-3}T\ln T - 9.678\times10^{-6}T^2 - 318.225T^{-1} + 8.961\times10^{-3}T$

544.59-681.8 K: $\Delta Hf° = -57.811 - 9.475\times10^{-3}T + 12.721\times10^{-6}T^2 - 335.850T^{-1}$

$\Delta Gf° = -57.811 + 9.475\times10^{-3}T\ln T - 12.721\times10^{-6}T^2 - 167.925T^{-1} - 0.729\times10^{-3}T$

681.8-1000 K: $\Delta Hf° = -61.309 + 16.735\times10^{-3}T - 0.261\times10^{-6}T^2 + 354.750T^{-1}$

$\Delta Gf° = -61.309 - 16.735\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 + 177.375T^{-1} + 165.821\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Cubicciotti (43). High-temperature data from Cubicciotti (48). Heat capacity at 298 K estimated.

$BiI_3(g)$

Bismuth Triiodide (ideal gas)

[Formation: $Bi(c,l) + 1.5I_2(c,l,g) = BiI_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.620	97.580	97.580	0	-3.900	-16.536	12.121
300	19.620	97.701	97.581	.036	-3.911	-16.614	12.103
386.8	19.715	102.702	98.192	1.745	-4.552	-20.212	11.420
386.8	19.715	102.702	98.192	1.745	-10.115	-20.212	11.420
400	19.730	103.364	98.352	2.005	-10.321	-20.553	11.230
458.4	19.759	106.056	99.165	3.159	-11.232	-21.979	10.479
458.4	19.759	106.056	99.165	3.159	-26.264	-21.979	10.479
500	19.780	107.773	99.811	3.981	-26.280	-21.587	9.435
544.59	19.793	109.463	100.533	4.863	-26.308	-21.169	8.495
544.59	19.793	109.463	100.533	4.863	-29.008	-21.169	8.495
600	19.810	111.382	101.449	5.960	-29.055	-20.373	7.421
700	19.820	114.437	103.091	7.942	-29.114	-18.920	5.907
800	19.830	117.084	104.679	9.924	-29.161	-17.456	4.769
900	19.840	119.420	106.189	11.908	-29.201	-15.996	3.884
1000*	19.840	121.510	107.618	13.892	-29.233	-14.520	3.173
1100	19.850	123.402	108.969	15.876	-29.263	-13.052	2.593
1200	19.850	125.129	110.244	17.862	-29.290	-11.571	2.107
1300	19.860	126.718	111.451	19.847	-29.318	-10.093	1.697
1400	19.860	128.190	112.595	21.833	-29.351	-8.615	1.345
1500	19.850	129.560	113.681	23.818	-29.385	-7.133	1.039

*BiI_3 begins to decompose appreciably above 900 K, mainly by $BiI_3(g) = BiI(g) + I_2(g)$; Trifonov (246).

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
544.59 K, melting point of Bi; $\Delta H°$ = 2.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 19.875 - 0.008\times10^{-3}T - 0.225\times10^{5}T^{-2}$

$H°- H°_{298} = 19.875\times10^{-3}T - 0.004\times10^{-6}T^{2} + 0.225\times10^{2}T^{-1} - 6.001$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -2.926 - 2.764\times10^{-3}T - 5.444\times10^{-6}T^{2} + 99.600T^{-1}$

$\Delta Gf° = -2.926 + 2.764\times10^{-3}T\ln T + 5.444\times10^{-6}T^{2} + 49.800T^{-1} - 63.578\times10^{-3}T$

386.8-458.4 K: $\Delta Hf° = -5.109 - 12.370\times10^{-3}T - 3.206\times10^{-6}T^{2} + 99.600T^{-1}$

$\Delta Gf° = -5.109 + 12.370\times10^{-3}T\ln T + 3.206\times10^{-6}T^{2} + 49.800T^{-1} - 114.301\times10^{-3}T$

458.4-544.59 K: $\Delta Hf° = -27.179 + 3.140\times10^{-3}T - 3.308\times10^{-6}T^{2} + 76.650T^{-1}$

$\Delta Gf° = -27.179 - 3.140\times10^{-3}T\ln T + 3.308\times10^{-6}T^{2} + 38.325T^{-1} + 28.894\times10^{-3}T$

544.59-1500 K: $\Delta Hf° = -29.955 + 0.610\times10^{-3}T - 0.265\times10^{-6}T^{2} + 377.250T^{-1}$

$\Delta Gf° = -29.955 - 0.610\times10^{-3}T\ln T + 0.265\times10^{-6}T^{2} + 188.625T^{-1} + 19.204\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Cubicciotti (43). Other data from Manley (154).

BrCl(g)

Bromine Monochloride (ideal gas)

[Formation: $0.5Br_2(l,g) + 0.5Cl_2(g) = BrCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.363	57.337	57.337	0	3.500	-0.228	0.167
300	8.369	57.389	57.339	.015	3.491	-.251	.183
332.6	8.448	58.256	57.387	.289	3.338	-.650	.427
332.6	8.448	58.256	57.387	.289	-.195	-.650	.427
400	8.611	59.833	57.668	.866	-.194	-.743	.406
500	8.744	61.771	58.303	1.734	-.193	-.881	.385
600	8.826	63.373	59.018	2.613	-.193	-1.018	.371
700	8.881	64.738	59.739	3.499	-.192	-1.155	.361
800	8.921	65.926	60.440	4.389	-.193	-1.292	.353
900	8.952	66.979	61.110	5.282	-.194	-1.431	.347
1000	8.977	67.923	61.744	6.179	-.194	-1.567	.343
1100	8.998	68.780	62.345	7.078	-.195	-1.705	.339
1200	9.016	69.563	62.915	7.978	-.196	-1.842	.335
1300	9.033	70.286	63.454	8.881	-.197	-1.979	.333
1400	9.048	70.956	63.967	9.785	-.198	-2.116	.330
1500	9.063	71.581	64.454	10.690	-.200	-2.254	.328
1600	9.076	72.166	64.918	11.597	-.201	-2.390	.326
1700	9.089	72.717	65.361	12.506	-.202	-2.527	.325
1800	9.102	73.236	65.783	13.415	-.204	-2.663	.323
1900	9.114	73.729	66.189	14.326	-.205	-2.798	.322
2000	9.126	74.197	66.578	15.238	-.207	-2.936	.321

Phase change: 332.6 K, boiling point of Br_2; $\Delta H^\circ = 7.065$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.871 + 0.146\times10^{-3}T - 0.491\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.871\times10^{-3}T + 0.073\times10^{-6}T^2 + 0.491\times10^{2}T^{-1} - 2.816$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = 4.811 - 4.588\times10^{-3}T + 0.079\times10^{-6}T^2 + 14.950T^{-1}$

$\Delta Gf^\circ = 4.811 + 4.588\times10^{-3}T\ln T - 0.079\times10^{-6}T^2 + 7.475T^{-1} - 43.100\times10^{-3}T$

332.6-2000 K: $\Delta Hf^\circ = -0.189 - 0.007\times10^{-3}T + 0.001\times10^{-6}T^2 - 0.750T^{-1}$

$\Delta Gf^\circ = -0.189 + 0.007\times10^{-3}T\ln T - 0.001\times10^{-6}T^2 - 0.375T^{-1} - 1.422\times10^{-3}T$

Source: Data from JANAF (60).

BrF(g)

Bromine Monofluoride (ideal gas)

[Formation: $0.5Br_2(l,g) + 0.5F_2(g) = BrF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.877	54.700	54.700	0	-14.000	-17.664	12.948
300	7.885	54.749	54.700	.015	-14.009	-17.686	12.884
332.6	8.006	55.569	54.745	.274	-14.167	-18.078	11.879
332.6	8.006	55.569	54.745	.274	-17.699	-18.078	11.879
400	8.255	57.072	55.014	.823	-17.706	-18.155	9.920
500	8.488	58.941	55.619	1.661	-17.711	-18.267	7.985
600	8.640	60.503	56.306	2.518	-17.713	-18.378	6.694
700	8.744	61.843	57.004	3.387	-17.715	-18.489	5.773
800	8.820	63.015	57.682	4.266	-17.714	-18.599	5.081
900	8.877	64.058	58.335	5.151	-17.714	-18.710	4.543
1000	8.922	64.995	58.954	6.041	-17.714	-18.821	4.113
1100	8.960	65.848	59.543	6.935	-17.714	-18.932	3.761
1200	8.992	66.629	60.101	7.833	-17.713	-19.042	3.468
1300	9.019	67.349	60.631	8.733	-17.713	-19.152	3.220
1400	9.044	68.019	61.136	9.636	-17.713	-19.264	3.007
1500	9.067	68.644	61.616	10.542	-17.713	-19.375	2.823
1600	9.087	69.229	62.073	11.450	-17.712	-19.484	2.661
1700	9.107	69.781	62.511	12.359	-17.712	-19.596	2.519
1800	9.125	70.302	62.929	13.271	-17.712	-19.707	2.393
1900	9.143	70.796	63.331	14.184	-17.711	-19.817	2.279
2000	9.160	71.265	63.715	15.099	-17.712	-19.928	2.178

Phase change: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.686 + 0.280\times10^{-3}T - 0.794\times10^{5}T^{-2}$

$H°- H°_{298} = 8.686\times10^{-3}T + 0.140\times10^{-6}T^{2} + 0.794\times10^{2}T^{-1} - 2.868$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -12.731 - 4.614\times10^{-3}T + 0.103\times10^{-6}T^{2} + 29.150T^{-1}$

$\Delta Gf° = -12.731 + 4.614\times10^{-3}T\ln T - 0.103\times10^{-6}T^{2} + 14.575T^{-1} - 42.963\times10^{-3}T$

332.6-2000 K: $\Delta Hf° = -17.732 - 0.033\times10^{-3}T + 0.025\times10^{-6}T^{2} + 13.450T^{-1}$

$\Delta Gf° = -17.732 + 0.033\times10^{-3}T\ln T - 0.025\times10^{-6}T^{2} + 6.725T^{-1} - 1.285\times10^{-3}T$

Source: Data from JANAF (60).

$BrF_3(g)$

Bromine Trifluoride (ideal gas)

[Formation: $0.5Br_2(l,g) + 1.5F_2(g) = BrF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	15.893	69.867	69.867	0	-61.100	-54.843	40.200
300	15.929	69.966	69.869	.029	-61.108	-54.805	39.925
332.6	16.391	71.633	69.962	.556	-61.245	-54.113	35.557
332.6	16.391	71.633	69.962	.556	-64.778	-54.113	35.557
400	17.345	74.763	70.513	1.700	-64.712	-51.958	28.388
500	18.145	78.727	71.771	3.478	-64.581	-48.784	21.323
600	18.627	82.081	73.216	5.319	-64.429	-45.638	16.623
700	18.936	84.978	74.695	7.198	-64.269	-42.519	13.275
800	19.145	87.521	76.142	9.103	-64.104	-39.424	10.770
900	19.291	89.785	77.535	11.025	-63.938	-36.348	8.826
1000	19.398	91.823	78.863	12.960	-63.773	-33.292	7.276
1100	19.478	93.676	80.127	14.904	-63.609	-30.252	6.010
1200	19.540	95.373	81.327	16.855	-63.446	-27.226	4.958
1300	19.588	96.939	82.469	18.811	-63.285	-24.213	4.071
1400	19.627	98.392	83.555	20.772	-63.127	-21.215	3.312
1500	19.658	99.748	84.591	22.736	-62.972	-18.229	2.656
1600	19.684	101.017	85.577	24.704	-62.817	-15.248	2.083
1700	19.705	102.211	86.521	26.673	-62.665	-12.280	1.579
1800	19.723	103.338	87.425	28.644	-62.518	-9.321	1.132
1900	19.738	104.405	88.291	30.617	-62.370	-6.368	.733
2000	19.751	105.417	89.121	32.592	-62.228	-3.424	.374

Phase change: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.232 + 0.386\times10^{-3}T - 3.070\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.232\times10^{-3}T + 0.193\times10^{-6}T^2 + 3.070\times10^{2}T^{-1} - 6.781$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -60.855 - 2.576\times10^{-3}T - 0.018\times10^{-6}T^2 + 156.250T^{-1}$

$\Delta Gf^\circ = -60.855 + 2.576\times10^{-3}T\ln T + 0.018\times10^{-6}T^2 + 78.125T^{-1} + 4.605\times10^{-3}T$

332.6-2000 K: $\Delta Hf^\circ = -65.855 + 2.005\times10^{-3}T - 0.095\times10^{-6}T^2 + 140.550T^{-1}$

$\Delta Gf^\circ = -65.855 - 2.005\times10^{-3}T\ln T + 0.095\times10^{-6}T^2 + 70.275T^{-1} + 46.283\times10^{-3}T$

Source: Data from JANAF (60).

$BrF_5(g)$

Bromine Pentafluoride (ideal gas)

[Formation: $0.5Br_2(l,g) + 2.5F_2(g) = BrF_5(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	24.236	77.337	77.337	0	-102.500	-84.027	61.592
300	24.304	77.487	77.337	.045	-102.507	-83.912	61.129
332.6	25.185	80.040	77.479	.852	-102.609	-81.887	53.807
332.6	25.185	80.040	77.479	.852	-106.142	-81.887	53.807
400	27.005	84.888	78.328	2.624	-105.971	-76.987	42.063
500	28.524	91.092	80.278	5.407	-105.639	-69.778	30.499
600	29.439	96.380	82.532	8.309	-105.256	-62.641	22.817
700	30.024	100.965	84.845	11.284	-104.848	-55.571	17.350
800	30.419	105.002	87.118	14.307	-104.427	-48.562	13.266
900	30.697	108.602	89.309	17.364	-103.997	-41.602	10.102
1000	30.899	111.847	91.403	20.444	-103.567	-34.695	7.583
1100	31.050	114.799	93.397	23.542	-103.135	-27.827	5.529
1200	31.167	117.506	95.295	26.653	-102.703	-21.000	3.825
1300	31.258	120.005	97.101	29.775	-102.271	-14.208	2.388
1400	31.331	122.324	98.821	32.904	-101.845	-7.453	1.163
1500	31.390	124.488	100.461	36.040	-101.421	-.726	.106
1600	31.439	126.515	102.026	39.182	-100.998	5.976	-.816
1700	31.479	128.422	103.523	42.328	-100.577	12.651	-1.626
1800	31.513	130.223	104.957	45.478	-100.163	19.297	-2.343
1900	31.542	131.927	106.332	48.630	-99.749	25.926	-2.982
2000	31.566	133.546	107.653	51.786	-99.343	32.527	-3.554

Phase change: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 30.597 + 0.722\times10^{-3}T - 5.846\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 30.597\times10^{-3}T + 0.361\times10^{-6}T^2 + 5.846\times10^{2}T^{-1} - 11.115$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -103.700 + 0.281\times10^{-3}T - 0.024\times10^{-6}T^2 + 333.350T^{-1}$

$\Delta Gf^\circ = -103.700 - 0.281\times10^{-3}T\ln T + 0.024\times10^{-6}T^2 + 166.675T^{-1} + 65.706\times10^{-3}T$

332.6-2000 K: $\Delta Hf^\circ = -108.700 + 4.862\times10^{-3}T - 0.101\times10^{-6}T^2 + 317.650T^{-1}$

$\Delta Gf^\circ = -108.700 - 4.862\times10^{-3}T\ln T + 0.101\times10^{-6}T^2 + 158.825T^{-1} + 107.384\times10^{-3}T$

Source: Data from JANAF (60).

CBr(g)

Carbon Monobromide (ideal gas)

[Formation: $C(c) + 0.5Br_2(l,g) = CBr(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.614	55.770	55.770	0	122.000	111.204	-81.514
300	8.621	55.823	55.770	.016	121.995	111.138	-80.963
332.6	8.704	56.717	55.819	.298	121.913	109.962	-72.255
332.6	8.704	56.717	55.819	.298	118.380	109.962	-72.255
400	8.876	58.344	56.112	.893	118.507	108.242	-59.140
500	8.973	60.337	56.765	1.786	118.643	105.659	-46.183
600	9.012	61.977	57.500	2.686	118.721	103.055	-37.537
700	9.031	63.367	58.241	3.588	118.753	100.440	-31.358
800	9.041	64.574	58.959	4.492	118.750	97.825	-26.724
900	9.049	65.639	59.643	5.396	118.718	95.209	-23.120
1000	9.056	66.593	60.292	6.301	118.666	92.599	-20.237
1100	9.062	67.456	60.904	7.207	118.597	90.007	-17.882
1200	9.069	68.245	61.483	8.114	118.514	87.401	-15.918
1300	9.076	68.971	62.032	9.021	118.419	84.811	-14.258
1400	9.083	69.644	62.552	9.929	118.315	82.230	-12.837
1500	9.090	70.271	63.046	10.837	118.201	79.656	-11.606
1600	9.098	70.858	63.516	11.747	118.082	77.091	-10.530
1700	9.105	71.410	63.965	12.657	117.955	74.531	-9.581
1800	9.113	71.930	64.392	13.568	117.824	71.982	-8.740
1900	9.121	72.423	64.802	14.480	117.688	69.440	-7.987
2000	9.129	72.891	65.195	15.392	117.545	66.904	-7.311

Phase change: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 9.177 - 0.050\times10^{-3}T - 0.487\times10^{5}T^{-2}$

$H°- H°_{298} = 9.177\times10^{-3}T - 0.025\times10^{-6}T^{2} + 0.487\times10^{2}T^{-1} - 2.897$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = 123.490 - 3.386\times10^{-3}T - 0.741\times10^{-6}T^{2} - 123.600T^{-1}$

$\Delta Gf° = 123.490 + 3.386\times10^{-3}T\ln T + 0.741\times10^{-6}T^{2} - 61.800T^{-1} - 60.027\times10^{-3}T$

332.6-2000 K: $\Delta Hf° = 118.490 + 1.194\times10^{-3}T - 0.819\times10^{-6}T^{2} - 139.300T^{-1}$

$\Delta Gf° = 118.490 - 1.194\times10^{-3}T\ln T + 0.819\times10^{-6}T^{2} - 69.650T^{-1} - 18.349\times10^{-3}T$

Source: Data from JANAF (60) who estimated some molecular constants.

CBr_4(c,l,g)
Carbon Tetrabromide
[Formation: $C(c) + 2Br_2(l,g) = CBr_4(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	35.134	50.800	50.800	0	4.450	11.406	-8.361
300	35.182	51.017	50.800	.065	4.445	11.450	-8.341
320	35.696	53.305	50.886	.774	4.390	11.918	-8.139
320	43.885	57.699	50.887	2.180	5.796	11.918	-8.139
332.6	43.386	59.384	51.177	2.730	5.863	12.158	-7.989
332.6	43.386	59.384	51.177	2.730	-8.267	12.158	-7.989
363	42.182	63.129	52.024	4.031	-7.569	13.993	-8.425
363	36.600	65.743	52.024	4.980	-6.620	13.993	-8.425
400	36.600	69.295	53.460	6.334	-6.014	16.059	-8.774
463	36.600	74.648	55.991	8.640	-5.010	19.457	-9.184
463	23.705	95.580	55.991	18.328	4.678	19.457	-9.184
500	24.005	97.414	58.992	19.211	4.782	20.633	-9.018
600	24.505	101.838	65.775	21.638	5.056	23.778	-8.661
700	24.829	105.642	71.205	24.106	5.314	26.877	-8.391
800	25.050	108.973	75.722	26.601	5.560	29.942	-8.180
900	25.206	111.933	79.584	29.114	5.788	32.973	-8.007
1000	25.321	114.595	82.955	31.640	6.007	35.981	-7.864
1100	25.407	117.012	85.942	34.177	6.216	38.981	-7.745
1200	25.473	119.226	88.625	36.721	6.416	41.940	-7.638
1300	25.525	121.267	91.059	39.271	6.606	44.891	-7.547
1400	25.567	123.160	93.284	41.826	6.790	47.831	-7.467
1500	25.600	124.925	95.336	44.384	6.964	50.755	-7.395

Phase changes: 320 K, transition point of CBr_4; ΔH° = 1.406 kcal/mol.
332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
363 K, melting point of CBr_4; ΔH° = 0.949 kcal/mol.
463 K, boiling point of CBr_4; ΔH° = 9.688 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-320 K: $Cp^\circ = 27.477 + 25.688\times10^{-3}T$
$H^\circ - H^\circ_{298} = 27.477\times10^{-3}T + 12.844\times10^{-6}T^2 - 9.334$

320-363 K: $Cp^\circ = 56.554 - 39.590\times10^{-3}T$
$H^\circ - H^\circ_{298} = 56.554\times10^{-3}T - 19.795\times10^{-6}T^2 - 13.890$

363-463 K: $Cp^\circ = 36.600$
$H^\circ - H^\circ_{298} = 36.600\times10^{-3}T - 8.306$

463-1500 K: $Cp^\circ = 25.605 + 0.128\times10^{-3}T - 4.201\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 25.605\times10^{-3}T + 0.064\times10^{-6}T^2 + 4.201\times10^{2}T^{-1} + 5.552$

CBr_4(c,l,g) - Continued

Formation equations (kcal/mol):

298.15-320 K: $\Delta Hf^\circ = 7.581 - 12.223\times10^{-3}T + 12.278\times10^{-6}T^2 - 172.300T^{-1}$

$\Delta Gf^\circ = 7.581 + 12.223\times10^{-3}T\ln T - 12.278\times10^{-6}T^2 - 86.150T^{-1} - 52.182\times10^{-3}T$

320-332.6 K: $\Delta Hf^\circ = 3.024 + 16.854\times10^{-3}T - 20.361\times10^{-6}T^2 - 172.300T^{-1}$

$\Delta Gf^\circ = 3.024 - 16.854\times10^{-3}T\ln T + 20.361\times10^{-6}T^2 - 86.150T^{-1} + 119.337\times10^{-3}T$

332.6-363 K: $\Delta Hf^\circ = -16.976 + 35.176\times10^{-3}T - 20.671\times10^{-6}T^2 - 235.100T^{-1}$

$\Delta Gf^\circ = -16.976 - 35.176\times10^{-3}T\ln T + 20.671\times10^{-6}T^2 - 117.550T^{-1} + 286.047\times10^{-3}T$

363-463 K: $\Delta Hf^\circ = -11.393 + 15.222\times10^{-3}T - 0.876\times10^{-6}T^2 - 235.100T^{-1}$

$\Delta Gf^\circ = -11.393 - 15.222\times10^{-3}T\ln T + 0.876\times10^{-6}T^2 - 117.550T^{-1} + 160.233\times10^{-3}T$

463-1500 K: $\Delta Hf^\circ = 2.465 + 4.227\times10^{-3}T - 0.812\times10^{-6}T^2 + 185.000T^{-1}$

$\Delta Gf^\circ = 2.465 - 4.227\times10^{-3}T\ln T + 0.812\times10^{-6}T^2 + 92.500T^{-1} + 61.869\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (202). Data 298-463 K based on Frederick (82). Data for gas from Kudchadker (136).

$CBr_4(g)$
Carbon Tetrabromide (ideal gas)
[Formation: $C(c) + 2Br_2(l,g) = CBr_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	21.782	85.526	85.526	0	19.000	15.602	-11.437
300	21.815	85.661	85.528	.040	18.970	15.582	-11.351
332.6	22.265	87.935	85.654	.759	18.442	15.240	-10.014
332.6	22.265	87.935	85.654	.759	4.312	15.240	-10.014
400	23.195	92.144	86.401	2.297	4.499	17.432	-9.524
500	24.005	97.414	88.092	4.661	4.782	20.633	-9.018
600	24.505	101.838	90.025	7.088	5.056	23.778	-8.661
700	24.829	105.642	91.991	9.556	5.314	26.877	-8.391
800	25.050	108.973	93.909	12.051	5.560	29.942	-8.180
900	25.206	111.933	95.751	14.564	5.788	32.973	-8.007
1000	25.321	114.595	97.505	17.090	6.007	35.981	-7.864
1100	25.407	117.012	99.169	19.627	6.216	38.981	-7.745
1200	25.473	119.226	100.750	22.171	6.416	41.940	-7.638
1300	25.525	121.267	102.251	24.721	6.606	44.891	-7.547
1400	25.567	123.160	103.677	27.276	6.790	47.831	-7.467
1500	25.600	124.925	105.036	29.834	6.964	50.755	-7.395

Phase change: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp^\circ = 24.942 + 0.606\times10^{-3}T - 2.970\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 24.942\times10^{-3}T + 0.303\times10^{-6}T^2 + 2.970\times10^{2}T^{-1} - 8.460$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = 23.005 - 14.758\times10^{-3}T - 0.263\times10^{-6}T^2 + 124.700T^{-1}$

$\Delta Gf^\circ = 23.005 + 14.758\times10^{-3}T\ln T + 0.263\times10^{-6}T^2 + 62.350T^{-1} - 109.695\times10^{-3}T$

332.6-1500 K: $\Delta Hf^\circ = 3.004 + 3.564\times10^{-3}T - 0.573\times10^{-6}T^2 + 61.900T^{-1}$

$\Delta Gf^\circ = 3.004 - 3.564\times10^{-3}T\ln T + 0.573\times10^{-6}T^2 + 30.950T^{-1} + 57.016\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Other data from Kudchadker (136).

CCl(g)

Carbon Monochloride (ideal gas)

[Formation: $C(c) + 0.5Cl_2(g) = CCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.709	53.634	53.634	0	120.000	112.362	-82.363
300	7.715	53.681	53.634	.014	120.003	112.315	-81.820
400	8.029	55.945	53.940	.802	120.132	109.732	-59.954
500	8.278	57.764	54.528	1.618	120.204	107.123	-46.823
600	8.459	59.291	55.199	2.455	120.229	104.503	-38.065
700	8.588	60.605	55.879	3.308	120.219	101.882	-31.809
800	8.684	61.758	56.543	4.172	120.181	99.265	-27.118
900	8.757	62.785	57.181	5.044	120.121	96.654	-23.470
1000	8.814	63.711	57.788	5.923	120.046	94.049	-20.554
1100	8.859	64.553	58.366	6.806	119.957	91.464	-18.172
1200	8.897	65.326	58.914	7.694	119.857	88.867	-16.185
1300	8.929	66.039	59.435	8.585	119.747	86.289	-14.506
1400	8.957	66.702	59.931	9.480	119.631	83.720	-13.069
1500	8.981	67.321	60.403	10.377	119.507	81.159	-11.825
1600	9.003	67.901	60.854	11.276	119.378	78.608	-10.737
1700	9.023	68.448	61.285	12.177	119.243	76.062	-9.778
1800	9.041	68.964	61.697	13.080	119.103	73.526	-8.927
1900	9.058	69.453	62.092	13.985	118.960	70.999	-8.167
2000	9.074	69.918	62.472	14.892	118.812	68.479	-7.483

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.391 + 0.432\times10^{-3}T - 0.720\times10^{5}T^{-2}$

$H°- H°_{298} = 8.391\times10^{-3}T + 0.216\times10^{-6}T^{2} + 0.720\times10^{2}T^{-1} - 2.762$

Formation equations (kcal/mol):

298.15 2000 K: $\Delta Hf° = 120.367 + 0.459\times10^{-3}T - 0.594\times10^{-6}T^{2} - 134.450T^{-1}$

$\Delta Gf° = 120.367 - 0.459\times10^{-3}T\ln T + 0.594\times10^{-6}T^{2} - 67.225T^{-1} - 23.650\times10^{-3}T$

Source: Data from JANAF (60).

$CCl_2(g)$

Carbon Dichloride (ideal gas)

[Formation: $C(c) + Cl_2(g) = CCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	11.054	63.392	63.392	0	57.000	54.397	-39.874
300	11.075	63.461	63.394	.020	57.001	54.380	-39.615
400	11.984	66.781	63.838	1.177	57.084	53.495	-29.228
500	12.559	69.522	64.710	2.406	57.143	52.590	-22.987
600	12.949	71.848	65.710	3.683	57.174	51.677	-18.823
700	13.259	73.868	66.735	4.993	57.182	50.759	-15.847
800	13.546	75.657	67.739	6.334	57.178	49.842	-13.616
900	13.835	77.269	68.710	7.703	57.170	48.925	-11.880
1000	14.132	78.742	69.641	9.101	57.167	48.008	-10.492
1100	14.428	80.103	70.531	10.529	57.174	47.102	-9.358
1200	14.713	81.371	71.383	11.986	57.193	46.175	-8.409
1300	14.975	82.559	72.197	13.471	57.226	45.256	-7.608
1400	15.206	83.677	72.977	14.980	57.272	44.333	-6.921
1500	15.401	84.733	73.726	16.511	57.329	43.407	-6.324
1600	15.557	85.732	74.445	18.059	57.395	42.478	-5.802
1700	15.677	86.679	75.137	19.621	57.466	41.544	-5.341
1800	15.762	87.578	75.804	21.193	57.540	40.604	-4.930
1900	15.816	88.432	76.447	22.772	57.615	39.662	-4.562
2000	15.843	89.244	77.067	24.355	57.685	38.715	-4.231

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 12.114 + 2.156\times10^{-3}T - 1.514\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 12.114\times10^{-3}T + 1.078\times10^{-6}T^2 + 1.514\times10^{2}T^{-1} - 4.215$

Formation equations (kcal/mol):

298.15 2000 K: $\Delta Hf^\circ = 57.348 - 0.231\times10^{-3}T + 0.224\times10^{-6}T^2 - 89.200T^{-1}$

$\Delta Gf^\circ = 57.348 + 0.231\times10^{-3}T\ln T - 0.224\times10^{-6}T^2 - 44.600T^{-1} - 10.645\times10^{-3}T$

Source: Data from JANAF (60) who estimated some molecular constants.

$CCl_3(g)$

Carbon Trichloride (ideal gas)

[Formation: $C(c) + 1.5Cl_2(g) = CCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	15.212	70.918	70.918	0	19.000	22.097	-16.198
300	15.245	71.012	70.919	.028	19.001	22.116	-16.112
400	16.658	75.606	71.536	1.628	19.113	23.138	-12.642
500	17.564	79.428	72.742	3.343	19.231	24.132	-10.548
600	18.156	82.686	74.134	5.131	19.339	25.103	-9.144
700	18.555	85.517	75.563	6.968	19.434	26.055	-8.135
800	18.834	88.014	76.966	8.838	19.517	26.994	-7.374
900	19.035	90.244	78.320	10.732	19.589	27.925	-6.781
1000	19.184	92.258	79.615	12.643	19.652	28.846	-6.304
1100	19.297	94.092	80.849	14.567	19.706	29.773	-5.915
1200	19.385	95.775	82.023	16.502	19.753	30.675	-5.587
1300	19.454	97.329	83.141	18.444	19.792	31.584	-5.310
1400	19.509	98.773	84.207	20.392	19.825	32.489	-5.072
1500	19.555	100.121	85.224	22.345	19.851	33.392	-4.865
1600	19.592	101.384	86.195	24.303	19.873	34.296	-4.685
1700	19.623	102.573	87.124	26.264	19.888	35.198	-4.525
1800	19.650	103.695	88.013	28.227	19.898	36.097	-4.383
1900	19.672	104.758	88.867	30.193	19.904	36.999	-4.256
2000	19.691	105.768	89.687	32.162	19.902	37.899	-4.141

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 18.503 + 0.836\times10^{-3}T - 3.148\times10^{5}T^{-2}$

$H°- H°_{298} = 18.503\times10^{-3}T + 0.418\times10^{-6}T^{2} + 3.148\times10^{2}T^{-1} - 6.610$

Formation equations (kcal/mol):

298.15 2000 K: $\Delta Hf° = 18.388 + 1.745\times10^{-3}T - 0.480\times10^{-6}T^{2} + 40.050T^{-1}$

$\Delta Gf° = 18.388 - 1.745\times10^{-3}T\ln T + 0.480\times10^{-6}T^{2} + 20.025T^{-1} + 22.012\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$CCl_4(l,g)$
Carbon Tetrachloride
[Formation: $C(c) + 2Cl_2(g) = CCl_4(l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	31.490	51.720	51.720	0	-32.370	-15.604	11.438
300	31.506	51.915	51.722	.058	-32.346	-15.501	11.292
350	31.818	56.793	52.108	1.640	-31.701	-12.746	7.959
350	21.080	77.322	52.108	8.825	-24.516	-12.746	7.959
400	21.918	80.180	55.405	9.910	-24.398	-11.057	6.041
500	23.088	85.207	60.877	12.165	-24.166	-7.747	3.386
600	23.823	89.486	65.298	14.513	-23.933	-4.485	1.633
700	24.306	93.197	69.024	16.921	-23.705	-1.262	.394
800	24.638	96.466	72.254	19.370	-23.487	1.928	-.527
900	24.874	99.382	75.109	21.846	-23.278	5.093	-1.237
1000	25.047	102.012	77.670	24.342	-23.077	8.232	-1.799
1100	25.178	104.406	79.993	26.854	-22.883	11.364	-2.258
1200	25.279	106.601	82.120	29.377	-22.698	14.459	-2.633
1300	25.359	108.628	84.083	31.909	-22.520	17.547	-2.950
1400	25.423	110.510	85.904	34.448	-22.348	20.622	-3.219
1500	25.474	112.265	87.603	36.993	-22.183	23.687	-3.451
1600	25.517	113.911	89.197	39.543	-22.023	26.740	-3.652
1700	25.552	115.459	90.697	42.096	-21.870	29.784	-3.829
1800	25.582	116.920	92.113	44.653	-21.722	32.818	-3.985
1900	25.608	118.304	93.455	47.213	-21.578	35.848	-4.123
2000	25.629	119.618	94.730	49.775	-21.444	38.866	-4.247

*Heat capacities extrapolated from 298 to 350 K.

Phase change: 350 K, boiling point of CCl_4; $\Delta H° = 7.185$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-350 K: $Cp° = 29.883 + 5.388\times10^{-3}T$

$H°- H°_{298} = 29.883\times10^{-3}T + 2.694\times10^{-6}T^2 - 9.149$

350-2000 K: $Cp° = 24.932 + 0.522\times10^{-3}T - 4.942\times10^{5}T^{-2}$

$H°- H°_{298} = 24.932\times10^{-3}T + 0.261\times10^{-6}T^2 + 4.942\times10^{2}T^{-1} - 1.345$

Formation equations (kcal/mol):

298.15-350 K: $\Delta Hf° = -34.087 + 8.711\times10^{-3}T + 1.752\times10^{-6}T^2 - 308.900T^{-1}$

$\Delta Gf° = -34.087 - 8.711\times10^{-3}T\ln T - 1.752\times10^{-6}T^2 - 154.450T^{-1} + 113.882\times10^{-3}T$

350-2000 K: $\Delta Hf° = -26.283 + 3.760\times10^{-3}T - 0.681\times10^{-6}T^2 + 185.300T^{-1}$

$\Delta Gf° = -26.283 - 3.760\times10^{-3}T\ln T + 0.681\times10^{-6}T^2 + 92.650T^{-1} + 59.714\times10^{-3}T$

Sources: Enthalpies of formation for liquid and gas at 298 K and entropy of liquid at 298 K from Wagman (252). Low-temperature heat capacities from Hicks (99) whose data was extrapolated to 350 K. Data for gas from JANAF (60).

$CCl_4(g)$

Carbon Tetrachloride (ideal gas)

[Formation: $C(c) + 2Cl_2(g) = CCl_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	19.933	74.019	74.019	0	-24.600	-14.483	10.616
300	19.979	74.142	74.019	.037	-24.597	-14.420	10.505
400	21.918	80.180	74.830	2.140	-24.398	-11.057	6.041
500	23.088	85.207	76.417	4.395	-24.166	-7.747	3.386
600	23.823	89.486	78.248	6.743	-23.933	-4.485	1.633
700	24.306	93.197	80.124	9.151	-23.705	-1.262	.394
800	24.638	96.466	81.966	11.600	-23.487	1.928	-.527
900	24.874	99.382	83.742	14.076	-23.278	5.093	-1.237
1000	25.047	102.012	85.440	16.572	-23.077	8.232	-1.799
1100	25.178	104.406	87.057	19.084	-22.883	11.364	-2.258
1200	25.279	106.601	88.595	21.607	-22.698	14.459	-2.633
1300	25.359	108.628	90.060	24.139	-22.520	17.547	-2.950
1400	25.423	110.510	91.454	26.678	-22.348	20.622	-3.219
1500	25.474	112.265	92.783	29.223	-22.183	23.687	-3.451
1600	25.517	113.911	94.053	31.773	-22.023	26.740	-3.652
1700	25.552	115.459	95.267	34.326	-21.870	29.784	-3.829
1800	25.582	116.920	96.429	36.883	-21.722	32.818	-3.985
1900	25.608	118.304	97.545	39.443	-21.578	35.848	-4.123
2000	25.629	119.618	98.615	42.005	-21.444	38.866	-4.247

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 24.505 + 0.794\times10^{-3}T - 4.275\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 24.505\times10^{-3}T + 0.397\times10^{-6}T^2 + 4.275\times10^{2}T^{-1} - 8.775$

Formation equations (kcal/mol):

298.15 2000 K: $\Delta Hf^\circ = -25.943 + 3.333\times10^{-3}T - 0.545\times10^{-6}T^2 + 118.600T^{-1}$

$\Delta Gf^\circ = -25.943 - 3.333\times10^{-3}T\ln T + 0.545\times10^{-6}T^2 + 59.300T^{-1} + 56.598\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Other data from JANAF (60).

$C_2Cl_2(g)$

Dichloroacetylene (ideal gas)

[Formation: $2C(c) + Cl_2(g) = C_2Cl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	15.672	64.989	64.989	0	50.100	47.430	-34.767
300	15.698	65.086	64.989	.029	50.106	47.413	-34.540
400	16.782	69.762	65.619	1.657	50.416	46.468	-25.388
500	17.507	73.590	66.842	3.374	50.646	45.453	-19.867
600	18.048	76.831	68.243	5.153	50.802	44.400	-16.172
700	18.478	79.647	69.676	6.980	50.903	43.323	-13.526
800	18.827	82.138	71.080	8.846	50.965	42.235	-11.538
900	19.115	84.373	72.436	10.743	50.998	41.139	-9.990
1000	19.352	86.399	73.732	12.667	51.014	40.043	-8.751
1100	19.549	88.253	74.969	14.612	51.014	38.967	-7.742
1200	19.713	89.962	76.149	16.576	51.002	37.850	-6.893
1300	19.850	91.545	77.273	18.554	50.978	36.755	-6.179
1400	19.966	93.020	78.345	20.545	50.947	35.662	-5.567
1500	20.064	94.401	79.370	22.546	50.906	34.571	-5.037
1600	20.148	95.699	80.351	24.557	50.861	33.485	-4.574
1700	20.220	96.923	81.290	26.576	50.807	32.399	-4.165
1800	20.282	98.080	82.191	28.601	50.747	31.320	-3.803
1900	20.335	99.178	83.056	30.632	50.682	30.244	-3.479
2000	20.382	100.223	83.889	32.668	50.607	29.169	-3.187

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 17.625 + 1.742\times10^{-3}T - 2.198\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 17.625\times10^{-3}T + 0.871\times10^{-6}T^2 + 2.198\times10^{2}T^{-1} - 6.070$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = 50.289 + 1.762\times10^{-3}T - 0.749\times10^{-6}T^2 - 193.100T^{-1}$

$\Delta Gf^\circ = 50.289 - 1.762\times10^{-3}T\ln T + 0.749\times10^{-6}T^2 - 96.550T^{-1} + 1.313\times10^{-3}T$

Source: Data from JANAF (60) who estimated some molecular constants.

$C_2Cl_4(g)$

Tetrachloroethylene (ideal gas)

[Formation: $2C(c) + 2Cl_2(g) = C_2Cl_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	22.836	82.052	82.052	0	-2.970	5.161	-3.783
300	22.887	82.194	82.054	.042	-2.966	5.211	-3.796
400	25.194	89.115	82.980	2.454	-2.702	7.898	-4.315
500	26.784	94.918	84.804	5.057	-2.439	10.518	-4.597
600	27.905	99.906	86.914	7.795	-2.193	13.088	-4.767
700	28.712	104.272	89.089	10.628	-1.964	15.614	-4.875
800	29.304	108.146	91.234	13.530	-1.752	18.110	-4.947
900	29.749	111.625	93.309	16.484	-1.552	20.580	-4.997
1000	30.089	114.777	95.301	19.476	-1.362	23.027	-5.032
1100	30.353	117.658	97.204	22.499	-1.181	25.479	-5.062
1200	30.562	120.308	99.021	25.545	-1.011	27.873	-5.076
1300	30.730	122.761	100.753	28.610	-.850	30.273	-5.089
1400	30.866	125.044	102.408	31.690	-.696	32.660	-5.098
1500	30.979	127.177	103.988	34.783	-.551	35.039	-5.105
1600	31.072	129.180	105.502	37.885	-.413	37.408	-5.110
1700	31.151	131.066	106.951	40.996	-.284	39.768	-5.112
1800	31.217	132.848	108.340	44.115	-.161	42.121	-5.114
1900	31.274	134.538	109.675	47.240	-.044	44.469	-5.115
2000	31.323	136.143	110.959	50.369	.059	46.809	-5.115

Phase change: 394.2 K, boiling point of C_2Cl_4; ΔH° = 8.3 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 27.936 + 2.282\times10^{-3}T - 5.139\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 27.936\times10^{-3}T + 1.141\times10^{-6}T^2 + 5.139\times10^{2}T^{-1} - 10.154$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -3.997 + 3.246\times10^{-3}T - 0.567\times10^{-6}T^2 + 32.700T^{-1}$

$\Delta Gf^\circ = -3.997 - 3.246\times10^{-3}T\ln T + 0.567\times10^{-6}T^2 + 16.350T^{-1} + 48.858\times10^{-3}T$

Sources: Boiling point data from Rossini (201). All other data from JANAF (60).

$C_2Cl_6(g)$
Hexachloroethane (ideal gas)
[Formation: $2C(c) + 3Cl_2(g) = C_2Cl_6(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	33.206	95.069	95.069	0	-32.080	-11.941	8.753
300	33.286	95.275	95.069	.062	-32.071	-11.817	8.608
400	36.677	105.355	96.423	3.573	-31.538	-5.144	2.810
500	38.781	113.782	99.074	7.354	-30.950	1.390	-.607
600	40.142	120.981	102.139	11.305	-30.360	7.804	-2.842
700	41.061	127.242	105.289	15.367	-29.780	14.116	-4.407
800	41.714	132.769	108.385	19.507	-29.216	20.346	-5.558
900	42.193	137.711	111.374	23.703	-28.664	26.508	-6.437
1000	42.551	142.176	114.235	27.941	-28.122	32.606	-7.126
1100	42.813	146.244	116.962	32.210	-27.592	38.675	-7.684
1200	43.024	149.979	119.561	36.502	-27.076	44.654	-8.133
1300	43.177	153.429	122.034	40.813	-26.571	50.611	-8.508
1400	43.296	156.633	124.393	45.136	-26.078	56.529	-8.824
1500	43.374	159.623	126.643	49.470	-25.598	62.413	-9.093
1600	43.435	162.424	128.792	53.811	-25.129	68.268	-9.325
1700	43.459	165.058	130.849	58.155	-24.676	74.092	-9.525
1800	43.478	167.543	132.820	62.502	-24.236	79.887	-9.699
1900	43.491	169.894	134.709	66.851	-23.807	85.665	-9.854
2000	43.500	172.125	136.525	71.200	-23.399	91.415	-9.989

Phase change: 457.6 K, sublimation point of C_2Cl_6; ΔH° = 12.2 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 41.043 + 1.872\times10^{-3}T - 7.463\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 41.043\times10^{-3}T + 0.936\times10^{-6}T^2 + 7.463\times10^{2}T^{-1} - 14.823$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -34.908 + 7.526\times10^{-3}T - 0.860\times10^{-6}T^2 + 196.800T^{-1}$

$\Delta Gf^\circ = -34.908 - 7.526\times10^{-3}T\ln T + 0.860\times10^{-6}T^2 + 98.400T^{-1} + 118.545\times10^{-3}T$

Sources: Sublimation data from Rossini (201). All other data from JANAF (60).

CF(g)

Carbon Monofluoride (ideal gas)

[Formation: $C(c) + 0.5F_2(g) = CF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	7.184	50.889	50.889	0	61.000	53.458	-39.185
300	7.188	50.934	50.891	.013	61.002	53.411	-38.909
400	7.432	53.033	51.173	.744	61.104	50.864	-27.791
500	7.709	54.721	51.719	1.501	61.142	48.299	-21.111
600	7.954	56.149	52.342	2.284	61.133	45.730	-16.657
700	8.154	57.391	52.977	3.090	61.091	43.165	-13.477
800	8.312	58.490	53.598	3.914	61.026	40.610	-11.094
900	8.438	59.477	54.198	4.751	60.940	38.061	-9.242
1000	8.538	60.371	54.771	5.600	60.842	35.524	-7.764
1100	8.619	61.189	55.318	6.458	60.733	33.008	-6.558
1200	8.686	61.942	55.839	7.324	60.615	30.482	-5.551
1300	8.742	62.639	56.335	8.195	60.489	27.976	-4.703
1400	8.789	63.289	56.809	9.072	60.357	25.479	-3.977
1500	8.829	63.897	57.262	9.953	60.219	22.992	-3.350
1600	8.864	64.468	57.695	10.837	60.075	20.515	-2.802
1700	8.895	65.006	58.109	11.725	59.927	18.047	-2.320
1800	8.923	65.515	58.506	12.616	59.775	15.589	-1.893
1900	8.947	65.998	58.887	13.510	59.621	13.139	-1.511
2000	8.970	66.458	59.255	14.406	59.460	10.696	-1.169

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 7.587 + 0.880\times10^{-3}T - 0.592\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 7.587\times10^{-3}T + 0.440\times10^{-6}T^2 + 0.592\times10^{2}T^{-1} - 2.500$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = 61.640 - 0.185\times10^{-3}T - 0.413\times10^{-6}T^2 - 163.350T^{-1}$

$\Delta Gf^\circ = 61.640 + 0.185\times10^{-3}T\ln T + 0.413\times10^{-6}T^2 - 81.675T^{-1} - 27.700\times10^{-3}T$

Source: Data from JANAF (60).

$CF_2(g)$
Carbon Difluoride (ideal gas)
[Formation: $C(c) + F_2(g) = CF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	9.309	57.533	57.533	0	-43.500	-45.801	33.573
300	9.327	57.591	57.534	.017	-43.501	-45.816	33.377
400	10.300	60.410	57.910	1.000	-43.531	-46.582	25.451
500	11.105	62.799	58.657	2.071	-43.581	-47.341	20.692
600	11.716	64.880	59.523	3.214	-43.645	-48.086	17.515
700	12.168	66.722	60.423	4.409	-43.722	-48.821	15.242
800	12.504	68.370	61.315	5.644	-43.808	-49.543	13.534
900	12.757	69.858	62.182	6.908	-43.902	-50.254	12.203
1000	12.950	71.213	63.020	8.193	-44.004	-50.957	11.136
1100	13.100	72.454	63.821	9.496	-44.111	-51.635	10.259
1200	13.219	73.599	64.589	10.812	-44.224	-52.325	9.530
1300	13.314	74.661	65.323	12.139	-44.342	-52.995	8.909
1400	13.391	75.651	66.027	13.474	-44.466	-53.658	8.376
1500	13.454	76.577	66.699	14.817	-44.594	-54.310	7.913
1600	13.507	77.447	67.344	16.165	-44.726	-54.952	7.506
1700	13.552	78.267	67.962	17.518	-44.863	-55.587	7.146
1800	13.591	79.043	68.557	18.875	-45.005	-56.214	6.825
1900	13.625	79.779	69.128	20.236	-45.149	-56.832	6.537
2000	13.655	80.478	69.678	21.600	-45.300	-57.442	6.277

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 11.451 + 1.472\times10^{-3}T - 2.294\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 11.451\times10^{-3}T + 0.736\times10^{-6}T^2 + 2.294\times10^{2}T^{-1} - 4.249$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -43.165 - 0.575\times10^{-3}T - 0.204\times10^{-6}T^2 - 43.400T^{-1}$

$\Delta Gf^\circ = -43.165 + 0.575\times10^{-3}T\ln T + 0.204\times10^{-6}T^2 - 21.700T^{-1} - 11.935\times10^{-3}T$

Source: Data from JANAF (60).

$CF_3(g)$

Carbon Trifluoride (ideal gas)

[Formation: $C(c) + 1.5F_2(g) = CF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	11.903	63.329	63.329	0	-112.400	-109.208	80.050
300	11.940	63.403	63.330	.022	-112.403	-109.188	79.543
400	13.735	67.092	63.820	1.309	-112.514	-108.097	59.061
500	15.133	70.315	64.803	2.756	-112.590	-106.984	46.762
600	16.172	73.170	65.965	4.323	-112.645	-105.858	38.558
700	16.936	75.724	67.180	5.981	-112.683	-104.724	32.696
800	17.503	78.024	68.394	7.704	-112.712	-103.585	28.298
900	17.928	80.111	69.581	9.477	-112.732	-102.442	24.876
1000	18.253	82.018	70.732	11.286	-112.750	-101.300	22.139
1100	18.506	83.770	71.838	13.125	-112.764	-100.143	19.896
1200	18.706	85.389	72.901	14.986	-112.778	-99.006	18.031
1300	18.865	86.893	73.920	16.865	-112.791	-97.857	16.451
1400	18.995	88.296	74.897	18.758	-112.807	-96.710	15.097
1500	19.102	89.610	75.835	20.663	-112.825	-95.559	13.923
1600	19.190	90.846	76.735	22.578	-112.843	-94.406	12.895
1700	19.265	92.011	77.599	24.501	-112.864	-93.251	11.988
1800	19.328	93.114	78.431	26.430	-112.890	-92.098	11.182
1900	19.382	94.161	79.232	28.366	-112.915	-90.941	10.461
2000	19.428	95.156	80.003	30.306	-112.949	-89.784	9.811

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 15.857 + 2.396\times10^{-3}T - 4.150\times10^{5}T^{-2}$

$H°- H°_{298} = 15.857\times10^{-3}T + 1.198\times10^{-6}T^{2} + 4.150\times10^{2}T^{-1} - 6.226$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -112.597 - 0.423\times10^{-3}T + 0.171\times10^{-6}T^{2} + 91.950T^{-1}$

$\Delta Gf° = -112.597 + 0.423\times10^{-3}T\ln T - 0.171\times10^{-6}T^{2} + 45.975T^{-1} + 8.494\times10^{-3}T$

Source: Data from JANAF (60).

$CF_4(g)$

Carbon Tetrafluoride (ideal gas)

[Formation: $C(c) + 2F_2(g) = CF_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	14.592	62.454	62.454	0	-223.040	-212.365	155.666
300	14.648	62.544	62.454	.027	-223.045	-212.299	154.658
400	17.304	67.139	63.062	1.631	-223.223	-208.685	114.019
500	19.290	71.225	64.295	3.465	-223.314	-205.040	89.622
600	20.741	74.877	65.759	5.471	-223.345	-201.381	73.352
700	21.799	78.158	67.301	7.600	-223.336	-197.722	61.731
800	22.580	81.122	68.846	9.821	-223.298	-194.065	53.015
900	23.166	83.817	70.361	12.110	-223.238	-190.413	46.238
1000	23.613	86.282	71.832	14.450	-223.165	-186.772	40.818
1100	23.960	88.550	73.251	16.829	-223.082	-183.126	36.383
1200	24.234	90.647	74.615	19.239	-222.992	-179.509	32.693
1300	24.453	92.595	75.923	21.674	-222.897	-175.886	29.569
1400	24.631	94.414	77.179	24.129	-222.801	-172.276	26.893
1500	24.777	96.119	78.386	26.599	-222.705	-168.672	24.575
1600	24.899	97.722	79.545	29.083	-222.607	-165.071	22.547
1700	25.001	99.234	80.659	31.578	-222.510	-161.477	20.759
1800	25.087	100.666	81.731	34.083	-222.416	-157.890	19.170
1900	25.161	102.024	82.763	36.595	-222.322	-154.306	17.749
2000	25.224	103.317	83.759	39.115	-222.234	-150.730	16.471

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 20.584 + 3.042\times10^{-3}T - 6.133\times10^{5}T^{-2}$

$H°- H°_{298} = 20.584\times10^{-3}T + 1.521\times10^{-6}T^2 + 6.133\times10^{2}T^{-1} - 8.329$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -223.896 + 0.050\times10^{-3}T + 0.407\times10^{-6}T^2 + 240.000T^{-1}$

$\Delta Gf° = -223.896 - 0.050\times10^{-3}T\ln T - 0.407\times10^{-6}T^2 + 120.000T^{-1} + 37.731\times10^{-3}T$

Source: Data from JANAF (60).

$C_2F_2(g)$

Difluoroacetylene (ideal gas)

[Formation: $2C(c) + F_2(g) = C_2F_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	13.608	58.305	58.305	0	5.000	2.878	-2.109
300	13.639	58.389	58.306	.025	5.003	2.864	-2.086
400	15.117	62.525	58.858	1.467	5.188	2.124	-1.161
500	16.242	66.025	59.951	3.037	5.320	1.341	-.586
600	17.111	69.066	61.223	4.706	5.405	.537	-.196
700	17.785	71.757	62.538	6.453	5.456	-.279	.087
800	18.310	74.167	63.845	8.258	5.481	-1.101	.301
900	18.722	76.349	65.115	10.111	5.489	-1.925	.467
1000	19.049	78.339	66.339	12.000	5.484	-2.750	.601
1100	19.311	80.167	67.513	13.919	5.469	-3.550	.705
1200	19.523	81.857	68.640	15.861	5.444	-4.391	.800
1300	19.696	83.426	69.717	17.822	5.410	-5.208	.876
1400	19.839	84.892	70.750	19.799	5.369	-6.027	.941
1500	19.958	86.264	71.738	21.789	5.320	-6.837	.996
1600	20.058	87.556	72.687	23.790	5.267	-7.645	1.044
1700	20.143	88.774	73.598	25.800	5.205	-8.451	1.086
1800	20.215	89.928	74.474	27.818	5.137	-9.252	1.123
1900	20.278	91.023	75.316	29.843	5.065	-10.050	1.156
2000	20.332	92.064	76.128	31.873	4.982	-10.842	1.185

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 16.524 + 2.482\times10^{-3}T - 3.250\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 16.524\times10^{-3}T + 1.241\times10^{-6}T^2 + 3.250\times10^{2}T^{-1} - 6.127$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = 5.152 + 0.980\times10^{-3}T - 0.465\times10^{-6}T^2 - 120.100T^{-1}$

$\Delta Gf^\circ = 5.152 - 0.980\times10^{-3}T\ln T + 0.465\times10^{-6}T^2 - 60.050T^{-1} - 1.507\times10^{-3}T$

Source: Data from JANAF (60) who estimated some molecular constants.

$C_2F_4(g)$

Tetrafluoroethylene (ideal gas)

[Formation: $2C(c) + 2F_2(g) = C_2F_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.230	71.678	71.678	0	-157.400	-149.066	109.267
300	19.287	71.797	71.678	.036	-157.400	-149.015	108.556
400	21.965	77.731	72.469	2.105	-157.357	-146.223	79.892
500	23.989	82.860	74.046	4.407	-157.297	-143.447	62.700
600	25.531	87.377	75.899	6.887	-157.231	-140.682	51.243
700	26.708	91.405	77.832	9.501	-157.161	-137.931	43.064
800	27.611	95.033	79.759	12.219	-157.085	-135.190	36.932
900	28.310	98.327	81.643	15.016	-157.004	-132.458	32.165
1000	28.858	101.339	83.463	17.876	-156.918	-129.737	28.354
1100	29.292	104.111	85.216	20.784	-156.830	-127.001	25.233
1200	29.641	106.675	86.898	23.732	-156.740	-124.315	22.641
1300	29.924	109.059	88.513	26.710	-156.652	-121.616	20.445
1400	30.157	111.286	90.061	29.715	-156.565	-118.927	18.565
1500	30.350	113.373	91.546	32.740	-156.482	-116.242	16.936
1600	30.512	115.337	92.972	35.784	-156.398	-113.558	15.511
1700	30.648	117.191	94.343	38.842	-156.320	-110.884	14.255
1800	30.764	118.946	95.661	41.913	-156.247	-108.212	13.139
1900	30.864	120.612	96.931	44.994	-156.176	-105.545	12.140
2000	30.950	122.198	98.156	48.085	-156.115	-102.883	11.242

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 24.712 + 4.104\times10^{-3}T - 5.961\times10^{5}T^{-2}$

$H°- H°_{298} = 24.712\times10^{-3}T + 2.052\times10^{-6}T^{2} + 5.961\times10^{2}T^{-1} - 9.550$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -157.781 + 0.660\times10^{-3}T + 0.172\times10^{-6}T^{2} + 50.500T^{-1}$

$\Delta Gf° = -157.781 - 0.660\times10^{-3}T\ln T - 0.172\times10^{-6}T^{2} + 25.250T^{-1} + 32.759\times10^{-3}T$

Source: Data from JANAF (60).

$C_2F_6(g)$
Hexafluoroethane (ideal gas)
[Formation: $2C(c) + 3F_2(g) = C_2F_6(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	25.432	79.368	79.368	0	-321.200	-300.716	220.428
300	25.528	79.526	79.369	.047	-321.203	-300.590	218.977
400	30.006	87.513	80.428	2.834	-321.211	-293.710	160.474
500	33.255	94.578	82.564	6.007	-321.084	-286.847	125.379
600	35.542	100.855	85.100	9.453	-320.882	-280.017	101.995
700	37.157	106.463	87.759	13.093	-320.634	-273.227	85.304
800	38.315	111.504	90.418	16.869	-320.362	-266.474	72.796
900	39.150	116.067	93.018	20.744	-320.074	-259.754	63.076
1000	39.791	120.226	95.534	24.692	-319.780	-253.071	55.308
1100	40.263	124.041	97.955	28.695	-319.483	-246.391	48.953
1200	40.652	127.562	100.277	32.742	-319.185	-239.782	43.670
1300	40.941	130.827	102.502	36.822	-318.890	-233.175	39.200
1400	41.185	133.870	104.636	40.928	-318.602	-226.597	35.373
1500	41.375	136.719	106.681	45.057	-318.318	-220.035	32.059
1600	41.541	139.394	108.642	49.203	-318.038	-213.488	29.161
1700	41.661	141.916	110.526	53.363	-317.766	-206.962	26.606
1800	41.771	144.301	112.337	57.535	-317.504	-200.452	24.338
1900	41.869	146.562	114.079	61.717	-317.245	-193.954	22.310
2000	41.957	148.712	115.758	65.908	-317.001	-187.473	20.486

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 35.746 + 4.274\times10^{-3}T - 10.301\times10^{5}T^{-2}$

$H°- H°_{298} = 35.746\times10^{-3}T + 2.137\times10^{-6}T^{2} + 10.301\times10^{2}T^{-1} - 14.303$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -323.445 + 3.186\times10^{-3}T + 0.083\times10^{-6}T^{2} + 384.000T^{-1}$

$\Delta Gf° = -323.445 - 3.186\times10^{-3}T\ln T - 0.083\times10^{-6}T^{2} + 192.000T^{-1} + 92.253\times10^{-3}T$

Source: Data from JANAF (60).

$CI_4(g)$

Carbon Tetraiodide (ideal gas)

[Formation: $C(c) + 2I_2(c,l,g) = CI_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	22.906	93.601	93.601	0	62.840	51.894	-38.039
300	22.933	93.743	93.603	.042	62.830	51.826	-37.755
386.8	23.856	99.698	94.325	2.078	62.243	48.713	-27.524
386.8	23.856	99.698	94.325	2.078	54.825	48.713	-27.524
400	23.996	100.501	94.516	2.394	54.594	48.508	-26.503
458.4	24.341	103.800	95.492	3.808	53.581	47.695	-22.739
458.4	24.341	103.800	95.492	3.808	33.539	47.695	-22.739
500	24.586	105.925	96.273	4.826	33.673	48.977	-21.408
600	24.938	110.441	98.268	7.304	33.980	52.008	-18.944
700	25.162	114.303	100.290	9.809	34.263	54.989	-17.168
800	25.312	117.674	102.258	12.333	34.526	57.933	-15.826
900	25.418	120.662	104.140	14.870	34.768	60.842	-14.774
1000	25.494	123.344	105.928	17.416	34.997	63.728	-13.928
1100	25.552	125.776	107.623	19.968	35.211	66.601	-13.232
1200	25.596	128.002	109.230	22.526	35.413	69.434	-12.646
1300	25.630	130.052	110.754	25.087	35.606	72.262	-12.148
1400	25.658	131.952	112.201	27.652	35.788	75.076	-11.720
1500	25.680	133.723	113.577	30.219	35.961	77.874	-11.346

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp^\circ = 25.351 + 0.332\times10^{-3}T - 2.262\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.351\times10^{-3}T + 0.166\times10^{-6}T^2 + 2.262\times10^{2}T^{-1} - 8.332$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = 64.147 - 3.921\times10^{-3}T - 3.584\times10^{-6}T^2 + 53.900T^{-1}$

$\Delta Gf^\circ = 64.147 + 3.921\times10^{-3}T\ln T + 3.584\times10^{-6}T^2 + 26.950T^{-1} - 64.808\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = 61.237 - 16.729\times10^{-3}T - 0.600\times10^{-6}T^2 + 53.900T^{-1}$

$\Delta Gf^\circ = 61.237 + 16.729\times10^{-3}T\ln T + 0.600\times10^{-6}T^2 + 26.950T^{-1} - 132.439\times10^{-3}T$

458.4-1500 K: $\Delta Hf^\circ = 31.810 + 3.951\times10^{-3}T - 0.736\times10^{-6}T^2 + 23.300T^{-1}$

$\Delta Gf^\circ = 31.810 - 3.951\times10^{-3}T\ln T + 0.736\times10^{-6}T^2 + 11.650T^{-1} + 58.487\times10^{-3}T$

Source: Data from Kudchadker (136).

CaBr(g)

Calcium Monobromide (ideal gas)

[Formation: $Ca(c,l,g) + 0.5Br_2(l,g) = CaBr(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.695	60.416	60.416	0	-11.800	-21.426	15.706
300	8.698	60.470	60.417	.016	-11.812	-21.485	15.652
332.6	8.740	61.369	60.467	.300	-12.020	-22.525	14.801
332.6	8.740	61.369	60.467	.300	-15.552	-22.525	14.801
400	8.828	62.992	60.760	.893	-15.672	-23.929	13.074
500	8.897	64.970	61.410	1.780	-15.869	-25.973	11.352
600	8.942	66.597	62.144	2.672	-16.104	-27.970	10.188
700	8.974	67.978	62.881	3.568	-16.387	-29.931	9.345
720	8.979	68.231	63.026	3.748	-16.451	-30.313	9.201
720	8.979	68.231	63.026	3.748	-16.671	-30.313	9.201
800	8.999	69.178	63.596	4.466	-16.903	-31.814	8.691
900	9.021	70.239	64.276	5.367	-17.261	-33.643	8.169
1000	9.040	71.190	64.920	6.270	-17.756	-35.455	7.749
1100	9.057	72.053	65.530	7.175	-18.329	-37.196	7.390
1112	9.059	72.151	65.601	7.284	-18.404	-37.407	7.352
1112	9.059	72.151	65.601	7.284	-20.444	-37.407	7.352
1200	9.073	72.841	66.106	8.082	-20.660	-38.740	7.055
1300	9.088	73.568	66.653	8.990	-20.904	-40.238	6.764
1400	9.103	74.242	67.171	9.899	-21.148	-41.714	6.512
1500	9.118	74.871	67.664	10.811	-21.390	-43.179	6.291
1600	9.132	75.460	68.133	11.723	-21.633	-44.627	6.096
1700	9.146	76.014	68.580	12.637	-21.874	-46.048	5.920
1757	9.155	76.316	68.827	13.158	-22.011	-46.857	5.828
1757	9.155	76.316	68.827	13.158	-58.637	-46.857	5.828
1800	9.161	76.537	69.008	13.552	-58.654	-46.536	5.650
1900	9.176	77.033	69.418	14.469	-58.692	-45.860	5.275
2000	9.193	77.504	69.810	15.388	-58.730	-45.185	4.938

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1757 K, boiling point of Ca; ΔH° = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.926 + 0.136\times10^{-3}T - 0.242\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.926\times10^{-3}T + 0.068\times10^{-6}T^2 + 0.242\times10^{2}T^{-1} - 2.748$

CaBr(g) - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -10.690 - 3.951\times10^{-3}T - 2.452\times10^{-6}T^2 + 85.200T^{-1}$

$\Delta Gf^\circ = -10.690 + 3.951\times10^{-3}T\ln T + 2.452\times10^{-6}T^2 + 42.600T^{-1} - 59.728\times10^{-3}T$

332.6-720 K: $\Delta Hf^\circ = -15.690 + 0.630\times10^{-3}T - 2.530\times10^{-6}T^2 + 69.500T^{-1}$

$\Delta Gf^\circ = -15.690 - 0.630\times10^{-3}T\ln T + 2.530\times10^{-6}T^2 + 34.750T^{-1} - 18.051\times10^{-3}T$

720-1112 K: $\Delta Hf^\circ = -17.431 + 4.568\times10^{-3}T - 4.901\times10^{-6}T^2 + 8.500T^{-1}$

$\Delta Gf^\circ = -17.431 - 4.568\times10^{-3}T\ln T + 4.901\times10^{-6}T^2 + 4.250T^{-1} + 8.627\times10^{-3}T$

1112-1757 K: $\Delta Hf^\circ = -17.679 - 2.539\times10^{-3}T + 0.040\times10^{-6}T^2 + 8.500T^{-1}$

$\Delta Gf^\circ = -17.679 + 2.539\times10^{-3}T\ln T - 0.040\times10^{-6}T^2 + 4.250T^{-1} - 35.502\times10^{-3}T$

1757-2000 K: $\Delta Hf^\circ = -57.850 - 0.509\times10^{-3}T + 0.033\times10^{-6}T^2 + 8.500T^{-1}$

$\Delta Gf^\circ = -57.850 + 0.509\times10^{-3}T\ln T - 0.033\times10^{-6}T^2 + 4.250T^{-1} + 2.516\times10^{-3}T$

Source: Data from Chase (26) who estimated some molecular constants.

$CaBr_2(c,l)$

Calcium Dibromide

[Formation: $Ca(c,l,g) + Br_2(l,g) = CaBr_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	17.670	31.000	31.000	0	-163.200	-158.633	116.279
300	17.690	31.109	31.000	.033	-163.211	-158.602	115.540
332.6	18.000	32.950	31.102	.615	-163.416	-158.091	103.880
332.6	18.000	32.950	31.102	.615	-170.481	-158.091	103.880
400	18.640	36.348	31.708	1.856	-170.246	-155.606	85.018
500	19.090	40.560	33.072	3.744	-169.883	-151.991	66.434
600	19.410	44.070	34.620	5.670	-169.529	-148.443	54.069
700	19.700	47.083	36.190	7.625	-169.199	-144.960	45.258
720	19.762	47.639	36.500	8.020	-169.137	-144.264	43.789
720	19.762	47.639	36.500	8.020	-169.357	-144.264	43.789
800	20.010	49.734	37.722	9.610	-169.075	-141.489	38.653
900	20.380	52.111	39.190	11.629	-168.765	-138.045	33.522
1000	20.800	54.279	40.592	13.687	-168.555	-134.662	29.430
1015	20.870	54.590	40.797	14.000	-168.525	-134.154	28.886
1015	27.000	61.437	40.797	20.950	-161.575	-134.154	28.886
1100	27.000	63.608	42.476	23.245	-160.926	-131.882	26.202
1112	27.000	63.901	42.706	23.569	-160.840	-131.571	25.858
1112	27.000	63.901	42.706	23.569	-162.880	-131.571	25.858
1200	27.000	65.958	44.337	25.945	-161.915	-129.131	23.518
1300	27.000	68.119	46.084	28.645	-160.820	-126.444	21.257
1400	27.000	70.120	47.731	31.345	-159.726	-123.838	19.332
1500	27.000	71.982	49.285	34.045	-158.634	-121.317	17.676
1600	27.000	73.725	50.759	36.745	-157.543	-118.868	16.236
1700	27.000	75.362	52.159	39.445	-156.453	-116.476	14.974
1757	27.000	76.252	52.926	40.984	-155.832	-115.146	14.323
1757	27.000	76.252	52.926	40.984	-192.458	-115.146	14.323
1800	27.000	76.905	53.491	42.145	-191.904	-113.228	13.748
1900	27.000	78.365	54.762	44.845	-190.615	-108.890	12.525
2000	27.000	79.750	55.978	47.545	-189.329	-104.625	11.433

*Data 298-1015 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1015 K, melting point of $CaBr_2$; ΔH° = 6.950 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1757 K, boiling point of Ca; ΔH° = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1015 K: $Cp^\circ = 18.459 + 2.290\times10^{-3}T - 1.307\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 18.459\times10^{-3}T + 1.145\times10^{-6}T^2 + 1.307\times10^{2}2T^{-1} - 6.044$

1015-2000 K: $Cp^\circ = 27.000$

$H^\circ - H^\circ_{298} = 27.000\times10^{-3}T - 6.455$

$CaBr_2$(c,l) - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -162.693 - 3.463\times10^{-3}T - 1.325\times10^{-6}T^2 + 191.700T^{-1}$

$\Delta Hf^\circ = -162.693 + 3.463\times10^{-3}T\ln T + 1.325\times10^{-6}T^2 + 95.850T^{-1} - 7.587\times10^{-3}T$

332.6-720 K: $\Delta Hf^\circ = -172.693 + 5.698\times10^{-3}T - 1.480\times10^{-6}T^2 + 160.300T^{-1}$

$\Delta Gf^\circ = -172.693 - 5.698\times10^{-3}T\ln T + 1.480\times10^{-6}T^2 + 80.150T^{-1} + 75.768\times10^{-3}T$

720-1015 K: $\Delta Hf^\circ = -174.434 + 9.636\times10^{-3}T - 3.852\times10^{-6}T^2 + 99.300T^{-1}$

$\Delta Gf^\circ = -174.434 - 9.636\times10^{-3}T\ln T + 3.852\times10^{-6}T^2 + 49.650T^{-1} + 102.447\times10^{-3}T$

1015-1112 K: $\Delta Hf^\circ = -174.845 + 18.177\times1^{-3}T - 4.997\times10^{-6}T^2 - 31.400T^{-1}$

$\Delta Gf^\circ = -174.845 - 18.177\times1^{-3}T\ln T + 4.997\times10^{-6}T^2 - 15.700T^{-1} + 160.879\times10^{-3}T$

1112-1757 K: $\Delta Hf^\circ = -175.093 + 11.070\times10^{-3}T - 0.055\times10^{-6}T^2 - 31.400T^{-1}$

$\Delta Gf^\circ = -175.093 - 11.070\times10^{-3}T\ln T + 0.055\times10^{-6}T^2 - 15.700T^{-1} + 116.749\times10^{-3}T$

1757-2000 K: $\Delta Hf^\circ = -215.264 + 13.100\times10^{-3}T - 0.062\times10^{-6}T^2 - 31.400T^{-1}$

$\Delta GF^\circ = -215.264 - 13.100\times10^{-3}T\ln T + 0.062\times10^{-6}T^2 - 15.700T^{-1} + 154.767\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Parker (187). Data 298-1015 K estimated using the one relative enthalpy value reported by Dworkin (66). Enthalpy of fusion and heat capacity of liquid also from Dworkin.

$CaBr_2(g)$

Calcium Dibromide (ideal gas)

[Formation: $Ca(c,l,g) + Br_2(l,g) = CaBr_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	14.433	75.200	75.200	0	-92.000	-100.611	73.749
300	14.438	75.289	75.200	.027	-92.017	-100.662	73.332
332.6	14.501	76.782	75.282	.499	-92.332	-101.586	66.751
332.6	14.501	76.782	75.282	.499	-99.397	-101.586	66.751
400	14.630	79.473	75.771	1.481	-99.421	-102.031	55.747
500	14.725	82.749	76.849	2.950	-99.477	-102.680	44.881
600	14.778	85.439	78.064	4.425	-99.574	-103.309	37.630
700	14.811	87.719	79.283	5.905	-99.719	-103.925	32.447
720	14.815	88.136	79.523	6.201	-99.756	-104.041	31.580
720	14.815	88.136	79.523	6.201	-99.976	-104.041	31.580
800	14.832	89.699	80.465	7.387	-100.098	-104.484	28.543
900	14.847	91.446	81.589	8.871	-100.323	-105.005	25.498
1000	14.858	93.011	82.655	10.356	-100.686	-105.525	23.062
1100	14.866	94.428	83.663	11.842	-101.129	-105.987	21.057
1112	14.867	94.589	83.780	12.020	-101.189	-106.045	20.842
1112	14.867	94.589	83.780	12.020	-103.229	-106.045	20.842
1200	14.872	95.722	84.615	13.329	-103.331	-106.264	19.353
1300	14.876	96.912	85.514	14.817	-103.448	-106.503	17.905
1400	14.880	98.015	86.369	16.304	-103.567	-106.732	16.661
1500	14.883	99.042	87.180	17.793	-103.686	-106.959	15.584
1600	14.886	100.002	87.951	19.281	-103.807	-107.175	14.639
1700	14.888	100.905	88.687	20.770	-103.928	-107.374	13.804
1757	14.889	101.396	89.092	21.619	-103.997	-107.489	13.370
1757	14.889	101.396	89.092	21.619	-140.623	-107.489	13.370
1800	14.889	101.756	89.390	22.259	-140.590	-106.646	12.948
1900	14.891	102.561	90.062	23.748	-140.512	-104.760	12.050
2000	14.892	103.325	90.706	25.237	-140.437	-102.883	11.242

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
720 K, α - β transition point of Ca; $\Delta H°$ = 0.220 kcal/mol.
1112 K, melting point of Ca; $\Delta H°$ = 2.040 kcal/mol.
1757 K, boiling point of Ca; $\Delta H°$ = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 14.880 + 0.014\times10^{-3}T - 0.402\times10^{5}T^{-2}$

$H°- H°_{298} = 14.880\times10^{-3}T + 0.007\times10^{-6}T^{2} + 0.402\times10^{2}T^{-1} - 4.572$

$CaBr_2(g)$ - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -90.021 - 7.042\times10^{-3}T - 2.463\times10^{-6}T^2 + 101.200T^{-1}$

$\Delta Gf^\circ = -90.021 + 7.042\times10^{-3}T\ln T + 2.463\times10^{-6}T^2 + 50.600T^{-1} - 76.945\times10^{-3}T$

332.6-720 K: $\Delta Gf^\circ = -100.021 + 2.119\times10^{-3}T - 2.618\times10^{-6}T^2 + 69.800T^{-1}$

$\Delta Gf^\circ = -100.021 - 2.119\times10^{-3}T\ln T + 2.618\times10^{-6}T^2 + 34.900T^{-1} + 6.410\times10^{-3}T$

720-1112 K: $\Delta Hf^\circ = -101.762 + 6.057\times10^{-3}T - 4.990\times10^{-6}T^2 + 8.800T^{-1}$

$\Delta Gf^\circ = -101.762 - 6.057\times10^{-3}T\ln T + 4.990\times10^{-6}T^2 + 4.400T^{-1} + 33.088\times10^{-3}T$

1112-1757 K: $\Delta Hf^\circ = -102.010 - 1.050\times10^{-3}T - 0.048\times10^{-6}T^2 + 8.800T^{-1}$

$\Delta Gf^\circ = -102.010 + 1.050\times10^{-3}T\ln T + 0.048\times10^{-6}T^2 + 4.400T^{-1} - 11.041\times10^{-3}T$

1757-2000 K: $\Delta Hf^\circ = -142.181 + 0.980\times10^{-3}T - 0.055\times10^{-6}T^2 + 8.800T^{-1}$

$\Delta Gf^\circ = -142.181 - 0.980\times10^{-3}T\ln T + 0.055\times10^{-6}T^2 + 4.400T^{-1} + 26.977\times10^{-3}T$

Source: Data from Chase (27).

CaCl(g)

Calcium Monochloride (ideal gas)

[Formation: $Ca(c,l,g) + 0.5Cl_2(g) = CaCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.524	57.707	57.707	0	-23.400	-29.698	21.769
300	8.529	57.760	57.707	.016	-23.402	-29.735	21.662
400	8.719	60.243	58.046	.879	-23.570	-31.823	17.387
500	8.822	62.200	58.686	1.757	-23.762	-33.865	14.802
600	8.885	63.815	59.412	2.642	-23.995	-35.863	13.063
700	8.928	65.188	60.141	3.533	-24.276	-37.824	11.809
720	8.935	65.440	60.285	3.712	-24.339	-38.207	11.597
720	8.935	65.440	60.285	3.712	-24.559	-38.207	11.597
800	8.961	66.382	60.847	4.428	-24.790	-39.708	10.848
900	8.987	67.439	61.522	5.325	-25.148	-41.537	10.086
1000	9.009	68.387	62.162	6.225	-25.642	-43.351	9.474
1100	9.028	69.247	62.768	7.127	-26.216	-45.093	8.959
1112	9.030	69.345	62.838	7.235	-26.292	-45.303	8.904
1112	9.030	69.345	62.838	7.235	-28.332	-45.303	8.904
1200	9.045	70.033	63.341	8.030	-28.549	-46.639	8.494
1300	9.061	70.758	63.884	8.936	-28.794	-48.137	8.092
1400	9.076	71.430	64.399	9.843	-29.039	-49.613	7.745
1500	9.091	72.056	64.889	10.751	-29.284	-51.078	7.442
1600	9.105	72.643	65.355	11.661	-29.528	-52.526	7.175
1700	9.119	73.196	65.801	12.572	-29.772	-53.946	6.935
1757	9.127	73.496	66.045	13.092	-29.910	-54.755	6.811
1757	9.127	73.496	66.045	13.092	-66.536	-54.755	6.811
1800	9.133	73.717	66.225	13.485	-66.554	-54.434	6.609
1900	9.147	74.212	66.634	14.399	-66.595	-53.760	6.184
2000	9.162	74.681	67.024	15.314	-66.638	-53.084	5.801

Phase changes: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1757 K, boiling point of Ca; ΔH° = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.906 + 0.136\times10^{-3}T - 0.376\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.906\times10^{-3}T + 0.068\times10^{-6}T^2 + 0.376\times10^{2}T^{-1} - 2.7872$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf^\circ = -23.587 + 0.661\times10^{-3}T - 2.546\times10^{-6}T^2 + 64.450T^{-1}$

$\Delta Gf^\circ = -23.587 - 0.661\times10^{-3}T\ln T + 2.546\times10^{-6}T^2 + 32.225T^{-1} - 17.847\times10^{-3}T$

720-1112 K: $\Delta Hf^\circ = -25.328 + 4.600\times10^{-3}T - 4.918\times10^{-6}T^2 + 3.450T^{-1}$

$\Delta Gf^\circ = -25.328 - 4.600\times10^{-3}T\ln T + 4.918\times10^{-6}T^2 + 1.725T^{-1} + 8.831\times10^{-3}T$

1112-1757 K: $\Delta Hf^\circ = -25.576 - 2.508\times10^{-3}T + 0.024\times10^{-6}T^2 + 3.450T^{-1}$

$\Delta Gf^\circ = -25.576 + 2.508\times10^{-3}T\ln T - 0.024\times10^{-6}T^2 + 1.725T^{-1} - 35.298\times10^{-3}T$

1757-2000 K: $\Delta Hf^\circ = -65.747 - 0.477\times10^{-3}T + 0.017\times10^{-6}T^2 + 3.450T^{-1}$

$\Delta Gf^\circ = -65.747 + 0.477\times10^{-3}T\ln T - 0.017\times10^{-6}T^2 + 1.725T^{-1} + 2.720\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (187). Other data from JANAF (60).

$CaCl_2(c,l)$
Calcium Dichloride
[Formation: $Ca(c,l,g) + Cl_2(g) = CaCl_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	17.360	25.000	25.000	0	-190.200	-178.802	131.064
300	17.377	25.107	25.000	.032	-190.194	-178.730	130.203
400	18.063	30.211	25.691	1.808	-189.864	-174.958	95.592
500	18.429	34.285	27.017	3.634	-189.534	-171.272	74.862
600	18.684	37.668	28.518	5.490	-189.231	-167.646	61.064
700	18.975	40.569	30.038	7.372	-188.959	-164.076	51.226
720	19.058	41.105	30.338	7.752	-188.909	-163.362	49.586
720	19.058	41.105	30.338	7.752	-189.129	-163.362	49.586
800	19.390	43.128	31.517	9.289	-188.894	-160.510	43.849
900	19.955	45.443	32.937	11.255	-188.628	-156.962	38.115
1000	20.637	47.580	34.296	13.284	-188.441	-153.473	33.541
1045	20.960	48.496	34.888	14.220	-188.358	-151.902	31.768
1045	25.516	54.936	34.888	20.950	-181.628	-151.902	31.768
1100	25.319	56.239	35.923	22.348	-181.301	-150.343	29.870
1112	25.276	56.513	36.143	22.652	-181.235	-150.011	29.482
1112	25.276	56.513	36.143	22.652	-183.275	-150.011	29.482
1200	24.961	58.427	37.709	24.862	-182.473	-147.410	26.847
1300	24.603	60.411	39.380	27.340	-181.597	-144.525	24.297
1400	24.244	62.221	40.947	29.783	-180.758	-141.702	22.120
1500	23.886	63.882	42.423	32.189	-179.958	-138.947	20.244
1600	23.528	65.412	43.812	34.560	-179.195	-136.240	18.609
1700	23.169	66.827	45.124	36.895	-178.469	-133.565	17.171
1757	22.965	67.588	45.840	38.210	-178.072	-132.069	16.428
1757	22.965	67.588	45.840	38.210	-214.698	-132.069	16.428
1800	22.811	68.141	46.367	39.194	-214.321	-130.018	15.786

Phase changes: 720 K, α - β transition point of Ca; $\Delta H°$ = 0.220 kcal/mol.
1045 K, melting point of CaCl2; $\Delta H°$ = 6.730 kcal/mol.
1112 K, melting point of Ca; $\Delta H°$ = 2.040 kcal/mol.
1757 K, boiling point of Ca; $\Delta H°$ = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1045 K: $Cp° = 16.692 + 3.678\times10^{-3}T - 0.381\times10^{5}T^{-2}$
$H°- H°_{298} = 16.692\times10^{-3}T + 1.839\times10^{-6}T^{2} + 0.381\times10^{2}T^{-1} - 5.268$

1045-1800 K: $Cp° = 29.223 - 3.562\times10^{-3}T + 0.168\times10^{5}T^{-2}$
$H°- H°_{298} = 29.223\times10^{-3}T - 1.781\times10^{-6}T^{2} - 0.168\times10^{2}T^{-1} - 7.627$

$CaCl_2$(c,l) - Continued

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf^\circ = -191.433 + 4.034\times10^{-3}T - 0.819\times10^{-6}T^2 + 30.800T^{-1}$

$\Delta Gf^\circ = -191.433 - 4.034\times10^{-3}T\ln T + 0.819\times10^{-6}T^2 + 15.400T^{-1} + 64.933\times10^{-3}T$

720-1045 K: $\Delta Hf^\circ = -193.174 + 7.972\times10^{-3}T - 3.191\times10^{-6}T^2 - 30.200T^{-1}$

$\Delta Gf^\circ = -193.174 - 7.972\times10^{-3}T\ln T + 3.191\times10^{-6}T^2 - 15.100T^{-1} + 91.611\times10^{-3}T$

1045-1112 K: $\Delta Hf^\circ = -195.533 + 20.503\times10^{-3}T - 6.811\times10^{-6}T2 - 85.100T^{-1}$

$\Delta Gf^\circ = -195.533 - 20.503\times10^{-3}T\ln T + 6.811\times10^{-6}T^2 - 42.550T^{-1} + 177.224\times10^{-3}T$

1112-1757 K: $\Delta Hf^\circ = -195.781 + 13.396\times10^{-3}T - 1.869\times10^{-6}T^2 - 85.100T^{-1}$

$\Delta Gf^\circ = -195.781 - 13.396\times10^{-3}T\ln T + 1.869\times10^{-5}T^2 - 42.550T^{-1} + 133.094\times10^{-3}T$

1757-1800 K: $\Delta Hf^\circ = -235.953 + 15.426\times10^{-3}T - 1.876\times10^{-6}T^2 - 85.100T^{-1}$

$\Delta Gf^\circ = -235.953 - 15.426\times10^{-3}T\ln T + 1.876\times10^{-6}T^2 - 42.550T^{-1} + 171.112\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (187). Low-temperature heat capacities and entropy at 298 K from Kelley (119). High-temperature data based on Moore (160).

$CaCl_2(g)$

Calcium Dichloride (ideal gas)

[Formation: $Ca(c,l,g) + Cl_2(g) = CaCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	14.179	69.347	69.347	0	-112.700	-114.524	83.947
300	14.187	69.435	69.348	.026	-112.700	-114.534	83.437
400	14.476	73.561	69.909	1.461	-112.711	-115.145	62.912
500	14.622	76.808	70.974	2.917	-112.751	-115.750	50.594
600	14.705	79.482	72.177	4.383	-112.838	-116.341	42.377
700	14.756	81.753	73.386	5.857	-112.974	-116.920	36.504
720	14.763	82.169	73.624	6.152	-113.009	-117.029	35.523
720	14.763	82.169	73.624	6.152	-113.229	-117.029	35.523
800	14.790	83.726	74.559	7.334	-113.349	-117.443	32.084
900	14.813	85.469	75.676	8.814	-113.569	-117.927	28.636
1000	14.830	87.031	76.734	10.297	-113.928	-118.411	25.878
1100	14.843	88.445	77.736	11.780	-114.369	-118.837	23.610
1112	14.844	88.606	77.852	11.958	-114.429	-118.891	23.366
1112	14.844	88.606	77.852	11.958	-116.469	-118.891	23.366
1200	14.853	89.737	78.683	13.265	-116.570	-119.079	21.687
1300	14.860	90.926	79.579	14.751	-116.686	-119.283	20.053
1400	14.866	92.028	80.430	16.237	-116.804	-119.478	18.651
1500	14.871	93.053	81.237	17.724	-116.923	-119.668	17.435
1600	14.875	94.013	82.006	19.211	-117.044	-119.850	16.371
1700	14.878	94.915	82.739	20.699	-117.165	-120.011	15.428
1757	14.880	95.406	83.143	21.547	-117.235	-120.109	14.940
1757	14.880	95.406	83.143	21.547	-153.861	-120.109	14.940
1800	14.881	95.766	83.440	22.187	-153.828	-119.250	14.479
1900	14.883	96.570	84.109	23.675	-153.751	-117.328	13.496
2000	14.885	97.334	84.753	25.163	-153.678	-115.416	12.612

Phase changes: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1757 K, boiling point of Ca; ΔH° = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 14.850 + 0.034\times10^{-3}T - 0.606\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.850\times10^{-3}T + 0.017\times10^{-6}T^2 + 0.606\times10^{2}T^{-1} - 4.632$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf^\circ = -113.298 + 2.192\times10^{-3}T - 2.641\times10^{-6}T^2 + 53.300T^{-1}$

$\Delta Gf^\circ = -113.298 - 2.192\times10^{-3}T\ln T + 2.641\times10^{-6}T2 + 26.650T^{-1} + 7.289\times10^{-3}T$

720-1112 K: $\Delta Hf^\circ = -115.039 + 6.130\times10^{-3}T - 5.013\times10^{-6}T^2 - 7.700T^{-1}$

$\Delta Gf^\circ = -115.039 - 6.130\times10^{-3}T\ln T + 5.013\times10^{-6}T^2 - 3.850T^{-1} + 33.967\times10^{-3}T$

1112-1757 K: $\Delta Hf^\circ = -115.287 - 0.977\times10^{-3}T - 0.071\times10^{-6}T^2 - 7.700T^{-1}$

$\Delta Gf^\circ = -115.287 + 0.977\times10^{-3}T\ln T + 0.071\times10^{-6}T^2 + 3.850T^{-1} - 10.162\times10^{-3}T$

1757-2000 K: $\Delta Hf^\circ = -155.458 + 1.053\times10^{-3}T - 0.078\times10^{-6}T^2 - 7.700T^{-1}$

$\Delta Gf^\circ = -155.458 - 1.053\times10^{-3}T\ln T + 0.078\times10^{-6}T^2 - 3.850T^{-1} + 27.856\times10^{-3}T$

Source: Data from JANAF (60).

CaF(g)

Calcium Monofluoride (ideal gas)

[Formation: $Ca(c,l,g) + 0.5F_2(g) = CaF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.045	54.860	54.860	0	-65.000	-71.171	52.169
300	8.053	54.910	54.860	.015	-65.003	-71.209	51.875
400	8.383	57.276	55.181	.838	-65.181	-73.251	40.022
500	8.579	59.169	55.795	1.687	-65.377	-75.248	32.890
600	8.702	60.745	56.492	2.552	-65.611	-77.198	28.119
700	8.784	62.093	57.199	3.426	-65.893	-79.113	24.700
720	8.796	62.341	57.338	3.602	-65.956	-79.487	24.127
720	8.796	62.341	57.338	3.602	-66.176	-79.487	24.127
800	8.844	63.270	57.885	4.308	-66.408	-80.951	22.114
900	8.888	64.314	58.543	5.194	-66.767	-82.733	20.090
1000	8.923	65.253	59.168	6.085	-67.264	-84.499	18.467
1100	8.952	66.105	59.760	6.979	-67.840	-86.194	17.125
1112	8.955	66.202	59.829	7.086	-67.916	-86.399	16.980
1112	8.955	66.202	59.829	7.086	-69.956	-86.399	16.980
1200	8.976	66.885	60.323	7.875	-70.175	-87.692	15.971
1300	8.997	67.604	60.855	8.774	-70.424	-89.141	14.986
1400	9.016	68.271	61.361	9.674	-70.674	-90.571	14.139
1500	9.033	68.894	61.843	10.577	-70.923	-91.988	13.402
1600	9.049	69.477	62.301	11.481	-71.172	-93.386	12.756
1700	9.064	70.026	62.740	12.387	-71.420	-94.756	12.182
1757	9.072	70.326	62.981	12.904	-71.562	-95.539	11.884
1757	9.072	70.326	62.981	12.904	-108.188	-95.539	11.884
1800	9.078	70.545	63.159	13.294	-108.209	-95.196	11.558
1900	9.092	71.036	63.561	14.202	-108.256	-94.472	10.867
2000	9.107	71.503	63.947	15.112	-108.305	-93.746	10.244

Phase changes: 720 K, α - β transition point of Ca; $\Delta H°$ = 0.220 kcal/mol.
1112 K, melting point of Ca; $\Delta H°$ = 2.040 kcal/mol.
1757 K, boiling point of Ca; $\Delta H°$ = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.767 + 0.204\times10^{-3}T - 0.696\times10^{5}T^{-2}$

$H°- H°_{298} = 8.767\times10^{-3}T + 0.102\times10^{-6}T^2 + 0.696\times10^{2}T^{-1} - 2.856$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf° = -65.246 + 0.682\times10^{-3}T - 2.555\times10^{-6}T^2 + 80.350T^{-1}$

$\Delta Gf° = -65.246 - 0.682\times10^{-3}T\ln T + 2.555\times10^{-6}T^2 + 40.175T^{-1} - 17.202\times10^{-3}T$

720-1112 K: $\Delta Hf° = -66.987 + 4.620\times10^{-3}T - 4.927\times10^{-6}T^2 + 19.350T^{-1}$

$\Delta Gf° = -66.987 - 4.620\times10^{-3}T\ln T + 4.927\times10^{-6}T^2 + 9.675T^{-1} + 9.476\times10^{-3}T$

1112-1757 K: $\Delta Hf° = -67.235 - 2.487\times10^{-3}T + 0.015\times10^{-6}T^2 + 19.350T^{-1}$

$\Delta Gf° = -67.235 + 2.487\times10^{-3}T\ln T - 0.015\times10^{-6}T^2 + 9.675T^{-1} - 34.654\times10^{-3}T$

1757-2000 K: $\Delta Hf° = -107.406 - 0.457\times10^{-3}T + 0.008\times10^{-6}T^2 + 19.350T^{-1}$

$\Delta Gf° = -107.406 + 0.457\times10^{-3}T\ln T - 0.008\times10^{-6}T^2 + 9.675T^{-1} + 3.364\times10^{-3}T$

Source: Data from JANAF (60).

$CaF_2(c,l)$

Calcium Difluoride

[Formation: $Ca(c,l,g) + F_2(g) = CaF_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	16.050	16.460	16.460	0	-293.800	-281.301	206.196
300	16.080	16.559	16.460	.030	-293.795	-281.222	204.867
400	17.472	21.385	17.108	1.711	-293.499	-277.073	151.384
500	18.480	25.400	18.376	3.512	-293.145	-273.008	119.330
600	19.095	28.829	19.841	5.393	-292.778	-269.014	97.987
700	19.505	31.804	21.341	7.324	-292.427	-265.086	82.763
720	19.593	32.355	21.639	7.715	-292.361	-264.303	80.226
720	19.593	32.355	21.639	7.715	-292.581	-264.303	80.226
800	19.945	34.436	22.817	9.295	-292.284	-261.175	71.349
900	20.524	36.817	24.243	11.317	-291.943	-257.291	62.478
1000	21.213	39.014	25.610	13.404	-291.684	-253.473	55.396
1100	22.037	41.073	26.924	15.564	-291.437	-249.662	49.603
1112	22.211	41.313	27.078	15.829	-291.408	-249.212	48.979
1112	22.211	41.313	27.078	15.829	-293.448	-249.212	48.979
1200	23.484	43.044	28.185	17.831	-292.847	-245.734	44.754
1300	27.136	45.045	29.405	20.332	-291.941	-241.843	40.657
1400	36.515	47.348	30.602	23.445	-290.428	-238.040	37.159
1430	41.323	48.170	30.960	24.610	-289.743	-236.923	36.209
1430	28.304	48.170	30.960	24.610	-289.743	-236.923	36.209
1500	29.081	49.542	31.796	26.619	-288.857	-234.363	34.146
1600	30.020	51.450	32.965	29.576	-287.506	-230.776	31.522
1690	30.726	53.112	33.994	32.310	-286.219	-227.610	29.434
1690	23.700	57.325	33.994	39.430	-279.099	-227.610	29.434
1700	23.700	57.465	34.131	39.667	-279.023	-227.306	29.222
1757	23.700	58.247	34.902	41.018	-278.591	-225.581	28.059
1757	23.700	58.247	34.902	41.018	-315.217	-225.581	28.059
1800	23.700	58.820	35.466	42.037	-314.805	-223.360	27.119

Phase changes: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1430 K, second order transition point of CaF_2: ΔH° = 0 kcal/mol.
1690 K, melting point of CaF_2; ΔH° = 7.120 kcal/mol.
1757 K, boiling point of Ca; ΔH° = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1430 K: $Cp^\circ = 9.813 + 13.256\times10^{-3}T + 2.031\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 9.813\times10^{-3}T + 6.628\times10^{-6}T^2 - 2.031\times10^{2}T^{-1} - 2.834$

1430-1690 K: $Cp^\circ = 36.832 - 174.389\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 36.832\times10^{-3}T + 174.389\times10^{2}T^{-1} - 40.255$

1690-1800 K: $Cp^\circ = 23.700$

$H^\circ - H^\circ_{298} = 23.700\times10^{-3}T - 0.623$

CaF_2(c,l) - Continued

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf^\circ = -292.578 - 2.526\times10^{-3}T + 3.884\times10^{-6}T^2 - 242.600T^{-1}$

$\Delta Gf^\circ = -292.578 + 2.526\times10^{-3}T\ln T - 3.884\times10^{-6}T^2 - 121.300T^{-1} + 25.956\times10^{-3}T$

720-1112 K: $\Delta Hf^\circ = -294.319 + 1.412\times10^{-3}T + 1.512\times10^{-6}T^2 - 303.600T^{-1}$

$\Delta Gf^\circ = -294.319 - 1.412\times10^{-3}T\ln T - 1.512\times10^{-6}T^2 - 151.800T^{-1} + 52.635\times10^{-3}T$

1112-1430 K: $\Delta Hf^\circ = -294.567 - 5.695\times10^{-3}T + 6.454\times10^{-6}T^2 - 303.600T^{-1}$

$\Delta Gf^\circ = -294.567 + 5.695\times10^{-3}T\ln T - 6.454\times10^{-6}T^2 - 151.800T^{-1} + 8.505\times10^{-3}T$

1430-1690 K: $\Delta Hf^\circ = -331.988 + 21.324\times10^{-3}T - 0.174\times10^{-6}T^2 + 17338.400T^{-1}$

$\Delta Gf^\circ = -331.988 - 21.324\times10^{-3}T\ln T + 0.174\times10^{-6}T^2 + 8669.200T^{-1} + 217.186\times10^{-3}T$

1690-1757 K: $\Delta Hf^\circ = -292.356 + 8.192\times10^{-3}T - 0.174\times10^{-6}T^2 - 100.500T^{-1}$

$\Delta Gf^\circ = -292.356 - 8.192\times10^{-3}T\ln T + 0.174\times10^{-6}T^2 - 50.250T^{-1} + 99.185\times10^{-3}T$

1757-1800 K: $\Delta Hf^\circ = -332.527 + 10.222\times10^{-3}T - 0.181\times10^{-6}T^2 - 100.500T^{-1}$

$\Delta Gf^\circ = -332.527 - 10.222\times10^{-3}T\ln T + 0.181\times10^{-6}T^2 - 50.250T^{-1} + 137.203\times10^{-3}T$

Sources: Enthalpy of formation of 298 K from Parker (188). Low-temperature heat capacities and entropy at 298 from Todd (238). High-temperature data based on Naylor (171).

$CaF_2(g)$

Calcium Difluoride (ideal gas)

[Formation: $Ca(c,l,g) + F_2(g) = CaF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.253	65.412	65.412	0	-189.100	-191.196	140.148
300	12.268	65.488	65.412	.023	-189.102	-191.208	139.293
400	12.875	69.110	65.903	1.283	-189.227	-191.891	104.843
500	13.209	72.022	66.844	2.589	-189.368	-192.542	84.159
600	13.408	74.449	67.916	3.920	-189.551	-193.159	70.357
700	13.534	76.526	69.000	5.268	-189.783	-193.748	60.490
720	13.551	76.908	69.215	5.539	-189.837	-193.857	58.843
720	13.551	76.908	69.215	5.539	-190.057	-193.857	58.843
800	13.619	78.339	70.056	6.626	-190.253	-194.267	53.070
900	13.678	79.947	71.068	7.991	-190.569	-194.734	47.287
1000	13.721	81.391	72.030	9.361	-191.027	-195.193	42.659
1100	13.753	82.700	72.941	10.735	-191.566	-195.581	38.858
1112	13.756	82.849	73.047	10.900	-191.638	-195.630	38.448
1112	13.756	82.849	73.047	10.900	-193.678	-195.630	38.448
1200	13.778	83.898	73.806	12.111	-193.867	-195.779	35.656
1300	13.797	85.001	74.624	13.490	-194.083	-195.928	32.938
1400	13.812	86.024	75.403	14.870	-194.303	-196.061	30.606
1500	13.825	86.978	76.143	16.252	-194.524	-196.184	28.584
1600	13.835	87.870	76.848	17.635	-194.747	-196.289	26.812
1700	13.843	88.709	77.521	19.019	-194.971	-196.368	25.245
1757	13.848	89.166	77.892	19.808	-195.100	-196.415	24.431
1757	13.848	89.166	77.892	19.808	-231.726	-196.415	24.431
1800	13.851	89.501	78.165	20.404	-231.738	-195.518	23.739
1900	13.857	90.250	78.782	21.789	-231.765	-193.505	22.258
2000	13.862	90.961	79.373	23.175	-231.796	-191.492	20.925

Phase changes: 720 K, α - β transition point of Ca; ΔH° = 0.220 kcal/mol.
1112 K, melting point of Ca; ΔH° = 2.040 kcal/mol.
1757 K, boiling point of Ca; ΔH° = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.676 + 0.146\times10^{-3}T - 1.303\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.676\times10^{-3}T + 0.073\times10^{-6}T^2 + 1.303\times10^{2}T^{-1} - 4.521$

Formation equations (kcal/mol):

298.15-720 K: $\Delta Hf^\circ = -189.566 + 1.337\times10^{-3}T - 2.671\times10^{-6}T^2 + 90.800T^{-1}$

$\Delta Gf^\circ = -189.566 - 1.337\times10^{-3}T\ln T + 2.671\times10^{-6}T^2 + 45.400T^{-1} + 0.844\times10^{-3}T$

720-1112 K: $\Delta Hf^\circ = -191.307 + 5.275\times10^{-3}T - 5.043\times10^{-6}T^2 + 29.800T^{-1}$

$\Delta Gf^\circ = -191.307 - 5.275\times10^{-3}T\ln T + 5.043\times10^{-6}T^2 + 14.900T^{-1} + 27.522\times10^{-3}T$

1112-1757 K: $\Delta Hf^\circ = -191.555 - 1.832\times10^{-3}T - 0.101\times10^{-6}T^2 + 29.800T^{-1}$

$\Delta Gf^\circ = -191.555 + 1.832\times10^{-3}T\ln T + 0.101\times10^{-6}T^2 + 14.900T^{-1} - 16.608\times10^{-3}T$

1757-2000 K: $\Delta Hf^\circ = -231.726 + 0.198\times10^{-3}T - 0.108\times10^{-6}T^2 + 29.800T^{-1}$

$\Delta Gf^\circ = -231.726 - 0.198\times10^{-3}T\ln T + 0.108\times10^{-6}T^2 + 14.900T^{-1} + 21.410\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (188). Other data from JANAF (60).

CaI(g)

Calcium Monoiodide (ideal gas)

[Formation: $Ca(c,l,g) + 0.5I_2(c,l,g) = CaI(g)$]

T, K	cal/mol-K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.758	62.426	62.426	0	-1.210	-12.721	9.324
300	8.761	62.481	62.428	.016	-1.217	-12.791	9.318
386.8	8.842	64.718	62.698	.781	-1.589	-16.092	9.092
386.8	8.842	64.718	62.698	.781	-3.444	-16.092	9.092
400	8.854	65.015	62.770	.898	-3.537	-16.523	9.027
458.4	8.882	66.225	63.135	1.416	-3.952	-18.390	8.768
458.4	8.882	66.225	63.135	1.416	-8.963	-18.390	8.768
500	8.902	66.997	63.425	1.786	-9.051	-19.241	8.410
600	8.932	68.623	64.161	2.677	-9.293	-21.256	7.742
700	8.953	70.001	64.898	3.572	-9.579	-23.232	7.253
720	8.956	70.253	65.043	3.751	-9.644	-23.618	7.169
720	8.956	70.253	65.043	3.751	-9.864	-23.618	7.169
800	8.970	71.198	65.613	4.468	-10.100	-25.131	6.865
900	8.983	72.255	66.294	5.365	-10.465	-26.975	6.550
1000	8.995	73.202	66.938	6.264	-10.966	-28.801	6.294
1100	9.005	74.060	67.547	7.164	-11.547	-30.555	6.071
1112	9.006	74.158	67.618	7.272	-11.623	-30.767	6.047
1112	9.006	74.158	67.618	7.272	-13.663	-30.767	6.047
1200	9.015	74.844	68.123	8.065	-13.886	-32.113	5.848
1300	9.024	75.566	68.668	8.967	-14.139	-33.622	5.652
1400	9.033	76.235	69.185	9.870	-14.392	-35.109	5.481
1500	9.042	76.858	69.675	10.774	-14.644	-36.584	5.330
1600	9.051	77.442	70.143	11.679	-14.896	-38.040	5.196
1700	9.060	77.991	70.589	12.584	-15.149	-39.470	5.074
1757	9.065	78.290	70.833	13.101	-15.292	-40.284	5.011
1757	9.065	78.290	70.833	13.101	-51.918	-40.284	5.011
1800	9.069	78.509	71.014	13.491	-51.941	-39.966	4.852
1900	9.079	79.000	71.422	14.398	-51.992	-39.300	4.520
2000	9.091	79.466	71.813	15.307	-52.043	-38.631	4.221

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
720 K, α - β transition point of Ca; $\Delta H°$ = 0.220 kcal/mol.
1112 K, melting point of Ca; $\Delta H°$ = 2.040 kcal/mol.
1757 K, boiling point of Ca; $\Delta H°$ = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.932 + 0.080\times10^{-3}T - 0.176\times10^{5}T^{-2}$

$H°- H°_{298} = 8.932\times10^{-3}T + 0.040\times10^{-6}T^{2} + 0.176\times10^{2}T^{-1} - 2.726$

CaI(g) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -0.784 - 1.338\times10^{-3}T - 3.276\times10^{-6}T^2 + 78.600T^{-1}$

$\Delta Gf^\circ = -0.784 + 1.338\times10^{-3}T\ln T + 3.276\times10^{-6}T^2 + 39.300T^{-1} - 49.076\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -1.511 - 4.539\times10^{-3}T - 2.530\times10^{-6}T^2 + 78.600T^{-1}$

$\Delta Gf^\circ = -1.511 + 4.539\times10^{-3}T\ln T + 2.530\times10^{-6}T^2 + 39.300T^{-1} - 65.984\times10^{-3}T$

458.4-720 K: $\Delta Hf^\circ = -8.868 + 0.630\times10^{-3}T - 2.564\times10^{-6}T^2 + 70.950T^{-1}$

$\Delta Gf^\circ = -8.868 - 0.630\times10^{-3}T\ln T + 2.564\times10^{-6}T^2 + 35.475T^{-1} - 18.253\times10^{-3}T$

720-1112 K: $\Delta Hf^\circ = -10.609 + 4.569\times10^{-3}T - 4.936\times10^{-6}T^2 + 9.950T^{-1}$

$\Delta Gf^\circ = -10.609 - 4.569\times10^{-3}T\ln T + 4.936\times10^{-6}T^2 + 4.975T^{-1} + 8.426\times10^{-3}T$

1112-1757 K: $\Delta Hf^\circ = -10.857 - 2.539\times10^{-3}T + 0.006\times10^{-6}T^2 + 9.950T^{-1}$

$\Delta Gf^\circ = -10.857 + 2.539\times10^{-3}T\ln T - 0.006\times10^{-6}T^2 + 4.975T^{-1} - 35.704\times10^{-3}T$

1757-2000 K: $\Delta Hf^\circ = -51.028 - 0.509\times10^{-3}T - 0.001\times10^{-6}T^2 + 9.950T^{-1}$

$\Delta Gf^\circ = -51.028 + 0.509\times10^{-3}T\ln T + 0.001\times10^{-6}T^2 + 4.975T^{-1} + 2.314\times10^{-3}T$

Source: Data from Chase (27).

CaI_2(c,l)

Calcium Diiodide

[Formation: $Ca(c,l,g) + I_2(c,l,g) = CaI_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.441	34.724	34.724	0	-128.300	-127.413	93.395
300*	18.450	34.839	34.726	.034	-128.301	-127.407	92.815
386.8	18.858	39.577	35.302	1.654	-128.423	-127.135	71.833
386.8	18.858	39.577	35.302	1.654	-132.132	-127.135	71.833
400	18.920	40.211	35.453	1.903	-132.220	-126.964	69.369
458.4	19.200	42.808	36.229	3.016	-132.603	-126.169	60.152
458.4	19.200	42.808	36.229	3.016	-142.624	-126.169	60.152
500	19.400	44.485	36.847	3.819	-142.465	-124.681	54.497
600	18.870	48.063	38.426	5.782	-142.083	-121.159	44.131
700	20.340	51.162	40.029	7.793	-141.703	-117.706	36.749
720	20.434	51.736	40.346	8.201	-141.629	-117.018	35.519
720	20.434	51.736	40.346	8.201	-141.849	-117.018	35.519
800	20.810	53.908	41.596	9.850	-141.513	-114.274	31.218
900	21.280	56.387	43.104	11.955	-141.122	-110.878	26.925
1000	21.750	58.653	44.547	14.106	-140.824	-107.552	23.505
1052	22.000	59.762	45.273	15.243	-140.680	-105.825	21.985
1052	24.700	69.268	45.273	25.243	-130.680	-105.825	21.985
1100	24.700	70.370	46.344	26.429	-130.435	-104.696	20.801
1112	24.700	70.638	46.604	26.725	-130.378	-104.421	20.522
1112	24.700	70.638	46.604	26.725	-132.418	-104.421	20.522
1200	24.700	72.519	48.436	28.899	-131.660	-102.235	18.619
1300	24.700	74.496	50.366	31.369	-130.799	-99.817	16.781
1400	24.700	76.326	52.155	33.839	-129.941	-97.464	15.215
1500	24.700	78.030	53.824	36.309	-129.084	-95.180	13.867
1600	24.700	79.624	55.387	38.779	-128.228	-92.948	12.696
1700	24.700	81.122	56.858	41.249	-127.374	-90.761	11.668
1757	24.700	81.937	57.659	42.657	-126.888	-89.544	11.138
1757	24.700	81.937	57.659	42.657	-163.514	-89.544	11.138
1800	24.700	82.534	58.246	43.719	-163.061	-87.706	10.649
1900	24.700	83.869	59.559	46.189	-162.009	-83.547	9.610
2000	24.700	85.136	60.807	48.659	-160.959	-79.445	8.681

*Data 300-1052 K estimated.

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
720 K, α - β transition point of Ca; $\Delta H°$ = 0.220 kcal/mol.
1052 K, melting point of CaI_2; $\Delta H°$ = 10.000 kcal/mol.
1112 K, melting point of Ca; $\Delta H°$ = 2.040 kcal/mol.
1757 K, boiling point of Ca; $\Delta H°$ = 36.626 kcal/mol.

CaI_2(c,1) - Continued

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1052 K: $Cp^\circ = 17.053 + 4.696\times10^{-3}T - 0.008\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 17.053\times10^{-3}T + 2.348\times10^{-6}T^2 + 0.008\times10^{2}T^{-1} - 5.296$

1052-2000 K: $Cp^\circ = 24.700$

$H^\circ - H^\circ_{298} = 24.700\times10^{-3}T - 0.741$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -128.458 + 0.345\times10^{-3}T - 1.714\times10^{-6}T^2 - 61.800T^{-1}$

$\Delta Gf^\circ = -128.458 - 0.345\times10^{-3}T\ln T + 1.714\times10^{-6}T^2 + 30.900T^{-1} + 4.610\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -129.913 - 6.059\times10^{-3}T - 0.222\times10^{-6}T^2 + 61.800T^{-1}$

$\Delta Gf^\circ = -129.913 + 6.059\times10^{-3}T\ln T + 0.222\times10^{-6}T^2 + 30.900T^{-1} - 29.205\times10^{-3}T$

458.4-720 K: $\Delta Hf^\circ = -144.626 + 4.281\times10^{-3}T - 0.290\times10^{-6}T^2 + 46.500T^{-1}$

$\Delta Gf^\circ = -144.626 - 4.281\times10^{-3}T\ln T + 0.290\times10^{-6}T^2 + 23.250T^{-1} + 66.258\times10^{-3}T$

720-1052 K: $\Delta Hf^\circ = -146.367 + 8.219\times10^{-3}T - 2.662\times10^{-6}T^2 - 14.500T^{-1}$

$\Delta Gf^\circ = -146.367 - 8.219\times10^{-3}T\ln T + 2.662\times10^{-6}T^2 - 7.250T^{-1} + 92.936\times10^{-3}T$

1052-1112 K: $\Delta Hf^\circ = -141.812 + 15.866\times10^{-3}T - 5.010\times10^{-6}T^2 - 15.300T^{-1}$

$\Delta Gf^\circ = -141.812 - 15.866\times10^{-3}T\ln T + 5.010\times10^{-6}T^2 - 7.650T^{-1} + 139.348\times10^{-3}T$

1112-1757 K: $\Delta Hf^\circ = -142.060 + 8.759\times10^{-3}T - 0.068\times10^{-6}T^2 - 15.300T^{-1}$

$\Delta Gf^\circ = -142.060 - 8.759\times10^{-3}T\ln T + 0.068\times10^{-6}T^2 - 7.650T^{-1} + 95.219\times10^{-3}T$

1757-2000 K: $\Delta Hf^\circ = -182.232 + 10.789\times10^{-3}T - 0.075\times10^{-6}T^2 - 15.300T^{-1}$

$\Delta Gf^\circ = -182.232 - 10.789\times10^{-3}T\ln T + 0.075\times10^{-6}T^2 - 7.650T^{-1} + 133.237\times10^{-3}T$

Source: Data from Chase (27) who estimated heat capacities 300-1052 K.

$CaI_2(g)$

Calcium Diiodide (ideal gas)

[Formation: $Ca(c,l,g) + I_2(c,l,g) = CaI_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	14.492	78.263	78.263	0	-61.700	-73.794	54.092
300	14.497	78.353	78.263	.027	-61.708	-73.868	53.812
386.8	14.643	82.058	78.717	1.293	-62.184	-77.328	43.691
386.8	14.643	82.058	78.717	1.293	-65.893	-77.328	43.691
400	14.665	82.550	78.835	1.486	-66.037	-77.716	42.462
458.4	14.713	84.552	79.439	2.344	-66.675	-79.376	37.843
458.4	14.713	84.552	79.439	2.344	-76.696	-79.376	37.843
500	14.748	85.832	79.918	2.957	-76.727	-79.617	34.800
600	14.794	88.525	81.135	4.434	-76.831	-80.184	29.207
700	14.823	90.808	82.358	5.915	-76.981	-80.737	25.207
720	14.827	91.226	82.599	6.211	-77.019	-80.840	24.538
720	14.827	91.226	82.599	6.211	-77.239	-80.840	24.538
800	14.842	92.789	83.540	7.399	-77.364	-81.230	22.191
900	14.855	94.538	84.667	8.884	-77.593	-81.685	19.836
1000	14.864	96.103	85.734	10.369	-77.961	-82.139	17.951
1100	14.871	97.520	86.742	11.856	-78.408	-82.534	16.398
1112	14.872	97.681	86.859	12.034	-78.468	-82.584	16.231
1112	14.872	97.681	86.859	12.034	-80.508	-82.584	16.231
1200	14.876	98.815	87.695	13.344	-80.615	-82.745	15.070
1300	14.880	100.005	88.597	14.831	-80.737	-82.917	13.939
1400	14.883	101.108	89.451	16.320	-80.860	-83.078	12.969
1500	14.886	102.135	90.263	17.808	-80.985	-83.238	12.128
1600	14.888	103.096	91.035	19.297	-81.110	-83.385	11.390
1700	14.890	103.999	91.772	20.786	-81.237	-83.515	10.736
1757	14.891	104.490	92.177	21.635	-81.310	-83.592	10.398
1757	14.891	104.490	92.177	21.635	-117.936	-83.592	10.398
1800	14.891	104.850	92.475	22.275	-117.905	-82.719	10.043
1900	14.893	105.655	93.148	23.764	-117.834	-80.765	9.290
2000	14.894	106.419	93.792	25.253	-117.765	-78.817	8.613

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
720 K, α - β transition point of Ca; $\Delta H°$ = 0.220 kcal/mol.
1112 K, melting point of Ca; $\Delta H°$ = 2.040 kcal/mol.
1757 K, boiling point of Ca; $\Delta H°$ = 36.626 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 14.887 + 0.010\times10^{-3}T - 0.354\times10^{5}T^{-2}$

$H°- H°_{298} = 14.887\times10^{-3}T + 0.005\times10^{-6}T^{2} + 0.354\times10^{2}T^{-1} - 4.558$

$CaI_2(g)$ - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -61.120 - 1.821\times10^{-3}T - 4.057\times10^{-6}T^2 + 96.400T^{-1}$

$\Delta Gf^\circ = -61.120 + 1.821\times10^{-3}T\ln T + 4.057\times10^{-6}T^2 + 48.200T^{-1} - 54.638\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -62.575 - 8.225\times10^{-3}T - 2.565\times10^{-6}T^2 + 96.400T^{-1}$

$\Delta Gf^\circ = -62.575 + 8.225\times10^{-3}T\ln T + 2.565\times10^{-6}T^2 + 48.200T^{-1} - 88.454\times10^{-3}T$

458.4-720 K: $\Delta Hf^\circ = -77.288 + 2.115\times10^{-3}T - 2.633\times10^{-6}T^2 + 81.100T^{-1}$

$\Delta Gf^\circ = -77.288 - 2.115\times10^{-3}T\ln T + 2.633\times10^{-6}T^2 + 40.550T^{-1} + 7.009\times10^{-3}T$

720-1112 K: $\Delta Hf^\circ = -79.029 + 6.053\times10^{-3}T - 5.005\times10^{-6}T^2 + 20.100T^{-1}$

$\Delta Gf^\circ = -79.029 - 6.053\times10^{-3}T\ln T + 5.005\times10^{-6}T^2 + 10.050T^{-1} + 33.687\times10^{-3}T$

1112-1757 K: $\Delta Hf^\circ = -79.277 - 1.054\times10^{-3}T - 0.063\times10^{-6}T^2 + 20.100T^{-1}$

$\Delta Gf^\circ = -79.277 + 1.054\times10^{-3}T\ln T + 0.063\times10^{-6}T^2 + 10.050T^{-1} - 10.442\times10^{-3}T$

1757-2000 K: $\Delta Hf^\circ = -119.448 + 0.976\times10^{-3}T - 0.070\times10^{-6}T^2 + 20.100T^{-1}$

$\Delta Gf^\circ = -119.448 - 0.976\times10^{-3}T\ln T + 0.070\times10^{-6}T^2 + 10.050T^{-1} + 27.576\times10^{-3}T$

Source: Data from Chase (27) who estimated most molecular constants.

$CdBr_2(c,l)$
Cadmium Dibromide
[Formation: $Cd(c,l) + Br_2(l,g) = CdBr_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	18.320	32.800	32.800	0	-75.570	-70.812	51.906
300*	18.330	32.913	32.800	.034	-75.580	-70.781	51.563
332.6	18.574	34.816	32.906	.636	-75.770	-70.250	46.160
332.6	18.574	34.816	32.906	.636	-82.835	-70.250	46.160
400	19.080	38.286	33.528	1.903	-82.588	-67.728	37.004
500	19.840	42.624	34.926	3.849	-82.188	-64.058	27.999
594.26	20.556	46.110	36.429	5.753	-81.771	-60.676	22.314
594.26	20.556	46.110	36.429	5.753	-83.251	-60.676	22.314
600	20.600	46.308	36.523	5.871	-83.227	-60.453	22.020
700	21.360	49.541	38.158	7.968	-82.733	-56.701	17.703
800	22.120	52.442	39.765	10.142	-82.164	-53.017	14.483
841.2	22.430	53.560	40.412	11.060	-81.908	-51.521	13.385
841.2	24.300	63.035	40.412	19.030	-73.938	-51.521	13.385
900	24.300	64.677	41.945	20.459	-73.456	-49.969	12.134
1000	24.300	67.237	44.348	22.889	-72.636	-47.401	10.359

*Data 300-800 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
594.26 K, melting point of Cd; ΔH° = 1.480 kcal/mol.
841.2 K, melting point of $CdBr_2$; ΔH° = 7.970 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-841.2 K: $Cp^\circ = 16.031 + 7.610\times10^{-3}T$
$H^\circ - H^\circ_{298} = 16.031\times10^{-3}T + 3.805\times10^{-6}T^2 - 5.118$

841.2-1000 K: $Cp^\circ = 24.300$
$H^\circ - H^\circ_{298} = 24.300\times10^{-3}T - 1.411$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -73.594 - 7.379\times10^{-3}T + 2.459\times10^{-6}T^2 + 1.600T^{-1}$
$\Delta Gf^\circ = -73.594 + 7.379\times10^{-3}T\ln T - 2.459\times10^{-6}T^2 + 0.800T^{-1} - 31.987\times10^{-3}T$

332.6-594.26 K: $\Delta Hf^\circ = -83.594 + 1.782\times10^{-3}T + 2.304\times10^{-6}T^2 - 29.800T^{-1}$
$\Delta Gf^\circ = -83.594 - 1.782\times10^{-3}T\ln T - 2.304\times10^{-6}T^2 - 14.900T^{-1} + 51.368\times10^{-3}T$

594.26-841.2 K: $\Delta Hf^\circ = -84.521 - 0.004\times10^{-3}T + 3.750\times10^{-6}T^2 - 31.400T^{-1}$
$\Delta Gf^\circ = -84.521 + 0.004\times10^{-3}T\ln T - 3.750\times10^{-6}T^2 - 15.700T^{-1} + 42.381\times10^{-3}T$

841.2-1000 K: $\Delta Hf^\circ = -80.814 + 8.265\times10^{-3}T - 0.055\times10^{-6}T^2 - 31.400T^{-1}$
$\Delta Gf^\circ = -80.814 - 8.265\times10^{-3}T\ln T + 0.055\times10^{-6}T^2 - 15.700T^{-1} + 90.464\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (252). Low-temperature heat capacities from Itskevich (106). High-temperature data estimated between 298 K and 841.2 K. Values at 841.2 K, enthalpy of fusion, and heat capacity of liquid based on Topol (243, 244).

$CdCl_2(c,l)$
Cadmium Dichloride
[Formation: $Cd(c,l) + Cl_2(g) = CdCl_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	17.840	27.550	27.550	0	-93.570	-82.205	60.257
300	17.855	27.660	27.550	.033	-93.563	-82.133	59.833
400	18.575	32.897	28.260	1.855	-93.206	-78.379	42.824
500	19.198	37.110	29.622	3.744	-92.834	-74.715	32.657
594.26	19.743	40.472	31.083	5.580	-92.467	-71.332	26.233
594.26	19.743	40.472	31.083	5.580	-93.947	-71.332	26.233
600	19.776	40.662	31.174	5.693	-93.927	-71.108	25.901
700	20.333	43.752	32.753	7.699	-93.509	-67.340	21.024
800	20.878	46.503	34.304	9.759	-93.045	-63.633	17.384
841	21.100	47.552	34.924	10.620	-92.839	-62.130	16.146
841	26.600	56.589	34.924	18.220	-85.239	-62.130	16.146
900	26.600	58.392	36.404	19.789	-84.615	-60.526	14.698
1000	26.600	61.195	38.746	22.449	-83.559	-57.906	12.655

Phase changes: 594.26 K, melting point of Cd; ΔHf° = 1.480 kcal/mol.
841 K, melting point of $CdCl_2$; ΔHf° = 7.600 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-841 K: $Cp^\circ = 16.750 + 5.246\times10^{-3}T - 0.438\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 16.750\times10^{-3}T + 2.623\times10^{-6}T^2 + 0.438\times10^{2}T^{-1} - 5.374$

841-1000 K: $Cp^\circ = 26.600$

$H^\circ - H^\circ_{298} = 26.600\times10^{-3}T - 4.151$

Formation equations (kcal/mol):

298.15-594.26 K: $\Delta Hf^\circ = -94.366 + 2.604\times10^{-3}T + 1.089\times10^{-6}T^2 - 22.900T^{-1}$

$\Delta Gf^\circ = -94.366 - 2.604\times10^{-3}T\ln T - 1.089\times10^{-6}T^2 - 11.450T^{-1} + 56.081\times10^{-3}T$

594.26-841 K: $\Delta Hf^\circ = -95.293 + 0.818\times10^{-3}T + 2.535\times10^{-6}T^2 - 24.500T^{-1}$

$\Delta Gf^\circ = -95.293 - 0.818\times10^{-3}T\ln T - 2.535\times10^{-6}T^2 - 12.250T^{-1} + 47.094\times10^{-3}T$

841-1000 K: $\Delta Hf^\circ = -94.070 + 10.668\times10^{-3}T - 0.088\times10^{-6}T^2 - 68.300T^{-1}$

$\Delta Gf^\circ = -94.070 - 10.668\times10^{-3}T\ln T + 0.088\times10^{-6}T^2 - 34.150T^{-1} + 109.800\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (252). Low-temperature heat capacities from Itskevich (105). High-temperature data based on Alim (3).

CdI_2(c,l)

Cadmium Diiodide

[Formation: $Cd(c,l) + I_2(c,l,g) = CdI_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	19.110	38.500	38.500	0	-48.600	-48.112	35.266
300*	19.122	38.618	38.501	.035	-48.600	-48.108	35.046
386.8	19.677	43.544	39.101	1.719	-48.674	-47.961	27.098
386.8	19.677	43.544	39.101	1.719	-52.383	-47.961	27.098
400	19.761	44.206	39.259	1.979	-52.463	-47.809	26.121
458.4	20.136	46.924	40.064	3.145	-52.807	-47.102	22.456
458.4	20.136	46.924	40.064	3.145	-62.828	-47.102	22.456
500	20.403	48.685	40.709	3.988	-62.636	-45.682	19.967
594.26	21.008	52.260	42.265	5.939	-62.180	-42.527	15.640
594.26	21.008	52.260	42.265	5.939	-63.660	-42.527	15.640
600	21.045	52.462	42.362	6.060	-63.634	-42.319	15.414
661.2	21.438	54.524	43.393	7.360	-63.318	-40.163	13.275
661.2	24.400	62.011	43.393	12.310	-58.368	-40.163	13.275
700	24.400	63.402	44.463	13.257	-58.046	-39.103	12.208
800	24.400	66.660	47.039	15.697	-57.217	-36.451	9.958
900	24.400	69.534	49.382	18.137	-56.391	-33.903	8.233
1000	24.400	72.105	51.528	20.577	-55.566	-31.446	6.872

*Data 300-600 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
594.26 K, melting point of Cd; ΔH° = 1.480 kcal/mol.
661.2 K, melting point of CdI_2; ΔH° = 4.950 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-661.2 K: $Cp^\circ = 17.195 + 6.418\times10^{-3}T$

$H^\circ - H^\circ_{298} = 17.195\times10^{-3}T + 3.209\times10^{-6}T^2 - 5.412$

661.2-1000 K: $Cp^\circ = 24.400$

$H^\circ - H^\circ_{298} = 24.400\times10^{-3}T - 3.823$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -48.331 - 1.001\times10^{-3}T + 0.271\times10^{-6}T^2 + 1.600T^{-1}$

$\Delta Gf^\circ = -48.331 + 1.001\times10^{-3}T\ln T - 0.271\times10^{-6}T^2 + 0.800T^{-1} - 4.896\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -49.786 - 7.405\times10^{-3}T + 1.763\times10^{-6}T^2 + 1.600T^{-1}$

$\Delta Gf^\circ = -49.786 + 7.405\times10^{-3}T\ln T - 1.763\times10^{-6}T^2 + 0.800T^{-1} - 38.711\times10^{-3}T$

458.4-594.26 K: $\Delta Hf^\circ = -64.499 + 2.935\times10^{-3}T + 1.695\times10^{-6}T^2 - 13.700T^{-1}$

$\Delta Gf^\circ = -64.499 - 2.935\times10^{-3}T\ln T - 1.695\times10^{-6}T^2 - 6.850T^{-1} + 56.752\times10^{-3}T$

594.26-661.2 K: $\Delta Hf^\circ = -65.426 + 1.149\times10^{-3}T + 3.141\times10^{-6}T^2 - 15.300T^{-1}$

$\Delta Gf^\circ = -65.426 - 1.149\times10^{-3}T\ln T - 3.141\times10^{-6}T^2 - 7.650T^{-1} + 47.765\times10^{-3}T$

661.2-1000 K: $\Delta Hf^\circ = -63.837 + 8.354\times10^{-3}T - 0.068\times10^{-6}T^2 - 15.300T^{-1}$

$\Delta Gf^\circ = -63.837 - 8.354\times10^{-3}T\ln T + 0.068\times10^{-6}T^2 - 7.650T^{-1} + 90.030\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Low-temperature heat capacities and entropy at 298 K from Dworkin (70). High-temperature data estimated between 298 K and 661.2 K. Values at 661.2 K, enthalpy of fusion, and heat capacity of liquid based on Topol (243, 244).

$CeBr_3(c,l)$
Cerium Tribromide
[Formation: $Ce(c,l) + 1.5Br_2(l,g) = CeBr_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	24.100	49.500	49.500	0	-211.000	-204.361	149.798
300	24.116	49.649	49.500	.045	-211.016	-204.318	148.844
332.6	24.375	52.150	49.638	.835	-211.320	-203.575	133.767
332.6	24.375	52.150	49.638	.835	-221.918	-203.575	133.767
400	24.911	56.702	50.457	2.498	-221.587	-199.893	109.215
500	25.572	62.333	52.287	5.023	-221.077	-194.531	85.028
600	26.183	67.050	54.365	7.611	-220.549	-189.267	68.940
700	26.771	71.131	56.475	10.259	-220.004	-184.102	57.478
800	27.347	74.743	58.537	12.965	-219.444	-179.003	48.901
900	27.915	77.997	60.521	15.728	-218.872	-173.985	42.249
999	28.473	80.939	62.400	18.520	-218.290	-169.081	36.989
999	28.473	80.939	62.400	18.520	-219.005	-169.081	36.989
1000	28.479	80.967	62.419	18.548	-218.999	-169.033	36.942
1005	28.507	81.109	62.512	18.690	-218.970	-168.784	36.704
1005	36.500	93.477	62.512	31.120	-206.540	-168.784	36.704
1071	36.500	95.799	64.493	33.529	-205.617	-166.329	33.941
1071	36.500	95.799	64.493	33.529	-206.922	-166.329	33.941
1100	36.500	96.774	65.331	34.587	-206.517	-165.235	32.829
1200	36.500	99.950	68.086	38.237	-205.122	-161.548	29.422
1300	36.500	102.872	70.651	41.887	-203.731	-157.976	26.558

*Heat capacity at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.
999 K, γ - δ transition point of Ce; $\Delta H° = 0.715$ kcal/mol.
1005 K, melting point of $CeBr_3$; $\Delta H° = 12.430$ kcal/mol.
1071 K, melting point of Ce; $\Delta H° = 1.305$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1005 K: $Cp° = 23.026 + 5.498\times10^{-3}T - 0.503\times10^{5}T^{-2}$
$H°-H°_{298} = 23.026\times10^{-3}T + 2.749\times10^{-6}T^2 + 0.503\times10^{2}T^{-1} - 7.278$

1005-1300 K: $Cp° = 36.500$
$H°-H°_{298} = 36.500\times10^{-3}T - 5.563$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -208.569 - 9.196\times10^{-3}T + 0.952\times10^{-6}T^2 + 67.500T^{-1}$
$\Delta Gf° = -208.569 + 9.196\times10^{-3}T\ln T - 0.952\times10^{-6}T^2 + 33.750T^{-1} - 38.372\times10^{-3}T$

332.6-999 K: $\Delta Hf° = -223.570 + 4.546\times10^{-3}T + 0.719\times10^{-6}T^2 + 20.400T^{-1}$
$\Delta Gf° = -223.570 - 4.546\times10^{-3}T\ln T - 0.719\times10^{-6}T^2 + 10.200T^{-1} + 86.661\times10^{-3}T$

999-1005 K: $\Delta Hf° = -222.310 + 0.641\times10^{-3}T + 2.667\times10^{-6}T^2 + 3.200T^{-1}$
$\Delta Gf° = -222.310 - 0.641\times10^{-3}T\ln T - 2.667\times10^{-6}T^2 + 1.600T^{-1} + 60.382\times10^{-3}T$

1005-1071 K: $\Delta Hf° = -220.595 + 14.115\times10^{-3}T - 0.083\times10^{-6}T^2 - 47.100T^{-1}$
$\Delta Gf° = -220.595 - 14.115\times10^{-3}T\ln T + 0.083\times10^{-6}T^2 - 23.550T^{-1} + 149.080\times10^{-3}T$

1071-1300 K: $\Delta Hf° = -221.878 + 14.095\times10^{-3}T - 0.083\times10^{-6}T^2 - 47.100T^{-1}$
$\Delta Gf° = -221.878 - 14.095\times10^{-3}T\ln T + 0.083\times10^{-6}T^2 - 23.550T^{-1} + 150.139\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Kim (122). Entropy at 298 K from Kelley (118). Heat capacity at 298 K estimated. High-temperature data based on Dworkin (69).

$CeBr_3(g)$

Cerium Tribromide (ideal gas)

[Formation: $Ce(c,l) + 1.5Br_2(l,g) = CeBr_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	19.135	95.186	95.186	0	-142.700	-149.682	109.718
300	19.144	95.304	95.187	.035	-142.726	-149.725	109.073
332.6	19.259	97.285	95.298	.661	-143.194	-150.461	98.866
332.6	19.259	97.285	95.298	.661	-153.792	-150.461	98.866
400	19.497	100.865	95.942	1.969	-153.816	-149.787	81.839
500	19.761	105.244	97.380	3.932	-153.868	-148.777	65.030
600	20.017	108.870	99.002	5.921	-153.938	-147.749	53.817
700	20.262	111.974	100.638	7.935	-154.028	-146.716	45.806
800	20.478	114.694	102.228	9.973	-154.136	-145.656	39.791
900	20.652	117.116	103.750	12.029	-154.271	-144.591	35.111
999	20.780	119.278	105.184	14.080	-154.429	-143.522	31.398
999	20.780	119.278	105.184	14.080	-155.144	-143.522	31.398
1000	20.781	119.299	105.198	14.101	-155.146	-143.512	31.364
1071	20.841	120.727	106.180	15.579	-155.266	-142.676	29.114
1071	20.841	120.727	106.180	15.579	-156.571	-142.676	29.114
1100	20.866	121.284	106.571	16.184	-156.620	-142.299	28.272
1200	20.915	123.102	107.874	18.273	-156.786	-140.994	25.678
1300	20.935	124.777	109.111	20.366	-156.952	-139.674	23.481
1400	20.932	126.329	110.286	22.460	-157.118	-138.334	21.595
1500	20.914	127.772	111.404	24.552	-157.289	-136.990	19.959
1600	20.885	129.121	112.470	26.642	-157.464	-135.632	18.526
1700	20.848	130.386	113.487	28.729	-157.643	-134.257	17.260
1800	20.807	131.577	114.460	30.811	-157.828	-132.886	16.134
1900	20.764	132.701	115.390	32.890	-158.018	-131.487	15.124
2000	20.721	133.765	116.283	34.964	-158.216	-130.093	14.216

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
999 K, γ - δ transition point of Ce; ΔH° = 0.715 kcal/mol.
1071 K, melting point of Ce; ΔH° = 1.305 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.915 + 0.730\times10^{-3}T - 0.887\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.915\times10^{-3}T + 0.365\times10^{-6}T^2 + 0.887\times10^{2}T^{-1} - 6.268$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -139.259 - 12.306\times10^{-3}T - 1.432\times10^{-6}T^2 + 105.900T^{-1}$

$\Delta Gf^\circ = -139.259 + 12.306\times10^{-3}T\ln T + 1.432\times10^{-6}T^2 + 52.950T^{-1} - 106.100\times10^{-3}T$

332.6-999 K: $\Delta Hf^\circ = -154.259 + 1.435\times10^{-3}T - 1.665\times10^{-6}T^2 + 58.800T^{-1}$

$\Delta Gf^\circ = -154.259 - 1.435\times10^{-3}T\ln T + 1.665\times10^{-6}T^2 + 29.400T^{-1} + 18.933\times10^{-3}T$

999-1071 K: $\Delta Hf^\circ = -152.999 - 2.470\times10^{-3}T + 0.282\times10^{-6}T^2 + 41.600T^{-1}$

$\Delta Gf^\circ = -152.999 + 2.470\times10^{-3}T\ln T - 0.282\times10^{-6}T^2 + 20.800T^{-1} - 7.346\times10^{-3}T$

1071-2000 K: $\Delta Hf^\circ = -154.283 - 2.490\times10^{-3}T + 0.282\times10^{-6}T^2 + 41.600T^{-1}$

$\Delta Gf^\circ = -154.283 + 2.490\times10^{-3}T\ln T - 0.282\times10^{-6}T^2 + 20.800T^{-1} - 6.287\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

$CeCl_3(c,l)$

Cerium Trichloride

[Formation: $Ce(c,l) + 1.5Cl_2(g) = CeCl_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	21.000	36.000	36.000	0	-251.800	-233.573	171.211
300	21.112	36.130	36.000	.039	-251.796	-233.460	170.073
400	24.827	42.802	36.884	2.367	-251.372	-227.402	124.245
500	26.332	48.525	38.657	4.934	-250.778	-221.479	96.807
600	27.125	53.402	40.719	7.610	-250.133	-215.676	78.559
700	27.719	57.628	42.838	10.353	-249.471	-209.990	65.561
800	28.327	61.369	44.925	13.155	-248.801	-204.390	55.836
900	29.052	64.745	46.943	16.022	-248.111	-198.881	48.294
999	29.938	67.821	48.861	18.941	-247.393	-193.507	42.333
999	29.938	67.821	48.861	18.941	-248.108	-193.507	42.333
1000	29.947	67.851	48.880	18.971	-248.101	-193.455	42.279
1071	30.709	69.931	50.208	21.123	-247.541	-189.589	38.687
1071	30.709	69.931	50.208	21.123	-248.846	-189.589	38.687
1080	30.806	70.188	50.373	21.400	-248.772	-189.091	38.264
1080	38.200	81.947	50.373	34.100	-236.072	-189.091	38.264
1100	38.200	82.648	50.953	34.864	-235.757	-188.224	37.396
1200	38.200	85.971	53.734	38.684	-234.188	-183.976	33.506
1300	38.200	89.029	56.334	42.504	-232.622	-179.858	30.236

Phase changes: 999 K, γ - δ transition point of Ce; ΔH° = 0.715 kcal/mol.
1071 K, melting point of Ce; ΔH° = 1.305 kcal/mol.
1080 K, melting point of $CeCl_3$; ΔH° = 12.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1080 K: $Cp^\circ = 27.582 + 2.648\times10^{-3}T - 6.555\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 27.582\times10^{-3}T + 1.324\times10^{-6}T^2 + 6.555\times10^{2}T^{-1} - 10.540$

1080-1300 K: $Cp^\circ = 38.200$

$H^\circ - H^\circ_{298} = 38.200\times10^{-3}T - 7.156$

Formation equations (kcal/mol):

298.15-999 K: $\Delta Hf^\circ = -256.405 + 9.257\times10^{-3}T - 0.755\times10^{-6}T^2 + 570.250T^{-1}$

$\Delta Gf^\circ = -256.405 - 9.257\times10^{-3}T\ln T + 0.755\times10^{-6}T^2 + 285.125T^{-1} + 125.889\times10^{-3}T$

999-1071 K: $\Delta Hf^\circ = -255.145 + 5.352\times10^{-3}T + 1.192\times10^{-6}T^2 + 553.050T^{-1}$

$\Delta Gf^\circ = -255.145 - 5.352\times10^{-3}T\ln T - 1.192\times10^{-6}T^2 + 276.525T^{-1} + 99.610\times10^{-3}T$

1071-1080 K: $\Delta Hf^\circ = -256.429 + 5.332\times10^{-3}T + 1.192\times10^{-6}T^2 + 553.050T^{-1}$

$\Delta Gf^\circ = -256.429 - 5.332\times10^{-3}T\ln T - 1.192\times10^{-6}T^2 + 276.525T^{-1} + 100.669\times10^{-3}T$

1080-1300 K: $\Delta Hf^\circ = -253.045 + 15.950\times10^{-3}T - 0.132\times10^{-6}T^2 - 102.450T^{-1}$

$\Delta Gf^\circ = -253.045 - 15.950\times10^{-3}T\ln T + 0.132\times10^{-6}T^2 - 51.225T^{-1} + 170.550\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (207). Entropy at 298 K from Westrum (261). Heat capacity at 298 K estimated. High-temperature data based on Walden (257).

$CeCl_3(g)$

Cerium Trichloride (ideal gas)

[Formation: $Ce(c,l) + 1.5Cl_2(g) = CeCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.737	88.576	88.576	0	-172.800	-170.248	124.794
300	18.750	88.692	88.576	.035	-172.799	-170.232	124.012
400	19.257	94.162	89.320	1.937	-172.803	-169.376	92.542
500	19.602	98.498	90.736	3.881	-172.831	-168.518	73.658
600	19.904	102.099	92.337	5.857	-172.886	-167.647	61.065
700	20.178	105.188	93.958	7.861	-172.963	-166.774	52.068
800	20.413	107.898	95.534	9.891	-173.064	-165.877	45.315
900	20.601	110.314	97.045	11.942	-173.191	-164.973	40.060
999	20.738	112.471	98.469	13.988	-173.346	-164.066	35.892
999	20.738	112.471	98.469	13.988	-174.061	-164.066	35.892
1000	20.739	112.492	98.483	14.009	-174.063	-164.057	35.854
1071	20.804	113.917	99.459	15.484	-174.180	-163.338	33.331
1071	20.804	113.917	99.459	15.484	-175.485	-163.338	33.331
1100	20.831	114.473	99.848	16.088	-175.533	-163.008	32.386
1200	20.886	116.288	101.143	18.174	-175.698	-161.867	29.480
1300	20.910	117.961	102.373	20.264	-175.862	-160.709	27.017
1400	20.911	119.511	103.543	22.355	-176.028	-159.535	24.904
1500	20.895	120.953	104.656	24.446	-176.197	-158.352	23.072
1600	20.868	122.301	105.717	26.534	-176.372	-157.160	21.467
1700	20.833	123.565	106.730	28.619	-176.551	-155.945	20.048
1800	20.794	124.754	107.698	30.701	-176.737	-154.736	18.787
1900	20.752	125.878	108.626	32.778	-176.929	-153.503	17.657
2000	20.710	126.941	109.516	34.851	-177.130	-152.270	16.639

Phase changes: 999 K, γ - δ transition point of Ce; $\Delta H° = 0.715$ kcal/mol.
1071 K, melting point of Ce; $\Delta H° = 1.305$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.879 + 0.752\times10^{-3}T - 1.215\times10^{5}T^{-2}$

$H°- H°_{298} = 19.879\times10^{-3}T + 0.376\times10^{-6}T^{2} + 1.215\times10^{2}T^{-1} - 6.368$

Formation equations (kcal/mol):

298.15-999 K: $\Delta Hf° = -173.233 + 1.554\times10^{-3}T - 1.703\times10^{-6}T^{2} + 36.250T^{-1}$

$\Delta Gf° = -173.233 - 1.554\times10^{-3}T\ln T + 1.703\times10^{-6}T^{2} + 18.125T^{-1} + 18.152\times10^{-3}T$

999-1071 K: $\Delta Hf° = -171.973 - 2.352\times10^{-3}T + 0.244\times10^{-6}T^{2} + 19.050T^{-1}$

$\Delta Gf° = -171.973 + 2.352\times10^{-3}T\ln T - 0.244\times10^{-6}T^{2} + 9.525T^{-1} - 8.127\times10^{-3}T$

1071-2000 K: $\Delta Hf° = -173.257 - 2.371\times10^{-3}T + 0.244\times10^{-6}T^{2} + 19.050T^{-1}$

$\Delta Gf° = -173.257 + 2.371\times10^{-3}T\ln T - 0.244\times10^{-6}T^{2} + 9.525T^{-1} - 7.068\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

CeF_3(c,l)

Cerium Trifluoride

[Formation: $Ce(c,l) + 1.5F_2(g) = CeF_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	22.250	27.600	27.600	0	-403.660	-385.096	282.279
300	22.279	27.738	27.601	.041	-403.652	-384.981	280.455
400	23.309	34.303	28.488	2.326	-403.181	-378.826	206.978
500	23.933	39.575	30.195	4.690	-402.716	-372.793	162.946
600	24.474	43.986	32.136	7.110	-402.268	-366.849	133.623
700	25.047	47.801	34.108	9.585	-401.829	-360.986	112.703
800	25.703	51.188	36.035	12.122	-401.387	-355.175	97.028
900	26.463	54.258	37.892	14.729	-400.930	-349.427	84.851
999	27.332	57.063	39.654	17.392	-400.447	-343.790	75.209
999	27.332	57.063	39.654	17.392	-401.162	-343.790	75.209
1000	27.341	57.090	39.671	17.419	-401.157	-343.734	75.122
1071	28.052	58.989	40.889	19.384	-400.773	-339.665	69.312
1071	28.052	58.989	40.889	19.384	-402.078	-339.665	69.312
1100	28.342	59.742	41.377	20.202	-401.907	-337.977	67.149
1200	29.472	62.256	43.014	23.091	-401.255	-332.200	60.501
1300	30.733	64.664	44.586	26.101	-400.489	-326.475	54.885
1400	32.127	66.991	46.104	29.242	-399.599	-320.813	50.080
1500	33.654	69.259	47.572	32.530	-398.566	-315.223	45.927
1600	35.316	71.483	48.997	35.978	-397.379	-309.705	42.303
1700	37.113	73.678	50.385	39.598	-396.022	-304.260	39.115
1710	37.301	73.896	50.522	39.970	-395.876	-303.720	38.817
1710	32.000	81.674	50.522	53.270	-382.576	-303.720	38.817
1800	32.000	83.315	52.121	56.150	-381.739	-299.601	36.376
1900	32.000	85.045	53.808	59.350	-380.809	-295.056	33.939
2000	32.000	86.687	55.412	62.550	-379.886	-290.574	31.752

Phase changes: 999 K, γ - δ transition point of Ce; $\Delta H°$ = 0.715 kcal/mol.
1071 K, melting point of Ce; $\Delta H°$ = 1.305 kcal/mol.
1710 K, melting point of CeF_3; $\Delta H°$ = 13.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1710 K: $Cp° = 17.635 + 10.368\times10^{-3}T + 1.354\times10^{5}T^{-2}$

$H°- H°_{298} = 17.635\times10^{-3}T + 5.184\times10^{-6}T^{2} - 1.354\times10^{2}T^{-1} - 5.265$

1710-2000 K: $Cp° = 32.000$

$H°- H°_{298} = 32.000\times10^{-3}T - 1.450$

CeF_3(c,l) - Continued

Formation equations (kcal/mol):

298.15-999 K: $\Delta Hf^\circ = -402.959 - 0.212\times10^{-3}T + 2.976\times10^{-6}T^2 - 268.950T^{-1}$

$\Delta Gf^\circ = -402.959 + 0.212\times10^{-3}T\ln T - 2.976\times10^{-6}T^2 - 134.475T^{-1} + 61.106\times10^{-3}T$

999-1071 K: $\Delta Hf^\circ = -401.699 - 4.117\times10^{-3}T + 4.923\times10^{-6}T^2 - 286.150T^{-1}$

$\Delta Gf^\circ = -401.699 + 4.117\times10^{-3}T\ln T - 4.923\times10^{-6}T^2 - 143.075T^{-1} + 34.828\times10^{-3}T$

1071-1710 K: $\Delta Hf^\circ = -402.983 - 4.137\times10^{-3}T + 4.923\times10^{-6}T^2 - 286.150T^{-1}$

$\Delta Gf^\circ = -402.983 + 4.137\times10^{-3}T\ln T - 4.923\times10^{-6}T^2 - 143.075T^{-1} + 35.887\times10^{-3}T$

1710-2000 K: $\Delta Hf^\circ = -399.167 + 10.228\times10^{-3}T - 0.261\times10^{-6}T^2 - 150.750T^{-1}$

$\Delta Gf^\circ = -399.167 - 10.228\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 - 75.375T^{-1} + 131.704\times10^{-3}T$

Sources: Enthalpy of formation from Afanas'ev (1). Low-temperature heat capacities and entropy at 298 K based on King (127) and Westrum (262). High-temperature data based on King (127).

$CeF_3(g)$

Cerium Trifluoride (ideal gas)

[Formation: $Ce(c,l) + 1.5F_2(g) = CeF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	17.345	80.543	80.543	0	-298.400	-295.621	216.693
300	17.368	80.651	80.544	.032	-298.401	-295.604	215.345
400	18.336	85.792	81.237	1.822	-298.424	-294.665	160.996
500	18.962	89.955	82.579	3.688	-298.458	-293.725	128.386
600	19.439	93.456	84.108	5.609	-298.508	-292.772	106.641
700	19.827	96.482	85.663	7.573	-298.581	-291.814	91.107
800	20.140	99.151	87.186	9.572	-298.677	-290.836	79.452
900	20.382	101.538	88.650	11.599	-298.800	-289.849	70.384
999	20.558	103.674	90.035	13.625	-298.953	-288.862	63.193
999	20.558	103.674	90.035	13.625	-299.668	-288.862	63.193
1000	20.560	103.695	90.049	13.646	-299.670	-288.852	63.128
1071	20.647	105.109	91.001	15.110	-299.787	-288.074	58.784
1071	20.647	105.109	91.001	15.110	-301.092	-288.074	58.784
1100	20.682	105.661	91.380	15.709	-301.140	-287.721	57.164
1200	20.760	107.464	92.646	17.781	-301.305	-286.499	52.178
1300	20.802	109.127	93.850	19.860	-301.470	-285.258	47.956
1400	20.818	110.670	94.998	21.941	-301.640	-284.004	44.334
1500	20.814	112.106	96.091	24.022	-301.814	-282.741	41.195
1600	20.796	113.448	97.134	26.103	-301.993	-281.464	38.446
1700	20.770	114.709	98.132	28.181	-302.178	-280.169	36.018
1800	20.737	115.895	99.086	30.257	-302.372	-278.878	33.860
1900	20.702	117.015	100.000	32.329	-302.570	-277.560	31.926
2000	20.664	118.076	100.877	34.397	-302.779	-276.244	30.186

Phase changes: 999 K, γ - δ transition point of Ce; $\Delta H°$ = 0.715 kcal/mol.
1071 K, melting point of Ce; $\Delta H°$ = 1.305 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.599 + 0.922\times10^{-3}T - 2.248\times10^{5}T^{-2}$

$H°-H°_{298} = 19.599\times10^{-3}T + 0.461\times10^{-6}T^{2} + 2.248\times10^{2}T^{-1} - 6.638$

Formation equations (kcal/mol):

298.15-999 K: $\Delta Hf° = -299.073 + 1.752\times10^{-3}T - 1.747\times10^{-6}T^{2} + 91.250T^{-1}$

$\Delta Gf° = -299.073 - 1.752\times10^{-3}T\ln T + 1.747\times10^{-6}T^{2} + 45.625T^{-1} + 20.527\times10^{-3}T$

999-1071 K: $\Delta Hf° = -297.813 - 2.153\times10^{-3}T + 0.200\times10^{-6}T^{2} + 74.050T^{-1}$

$\Delta Gf° = -297.813 + 2.153\times10^{-3}T\ln T - 0.200\times10^{-6}T^{2} + 37.025T^{-1} - 5.751\times10^{-3}T$

1071-2000 K: $\Delta Hf° = -299.096 - 2.173\times10^{-3}T + 0.200\times10^{-6}T^{2} + 74.050T^{-1}$

$\Delta Gf° = -299.096 + 2.173\times10^{-3}T\ln T - 0.200\times10^{-6}T^{2} + 37.025T^{-1} - 4.692\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

$CeI_3(c,l)$

Cerium Triiodide

[Formation: $Ce(c,l) + 1.5I_2(c,l,g) = CeI_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	24.000	54.300	54.300	0	-155.300	-153.947	112.845
300	24.000	54.449	54.302	.044	-155.304	-153.939	112.143
386.8	24.694	60.638	55.055	2.159	-155.572	-153.512	86.737
386.8	24.694	60.638	55.055	2.159	-161.135	-153.512	86.737
400	24.800	61.468	55.253	2.486	-161.280	-153.250	83.731
458.4	25.209	64.879	56.265	3.948	-161.906	-152.032	72.483
458.4	25.209	64.879	56.265	3.948	-176.937	-152.032	72.483
500	25.500	67.081	57.075	5.003	-176.733	-149.779	65.467
600	26.200	71.794	59.146	7.589	-176.219	-144.434	52.609
700	26.900	75.883	61.252	10.242	-175.679	-139.183	43.454
800	27.500	79.511	63.311	12.960	-175.115	-134.000	36.607
900	28.100	82.787	65.296	15.742	-174.533	-128.898	31.300
999	28.793	85.755	67.178	18.558	-173.933	-123.912	27.108
999	28.793	85.755	67.178	18.558	-174.648	-123.912	27.108
1000	28.800	85.784	67.197	18.587	-174.642	-123.863	27.070
1033	29.000	86.721	67.805	19.540	-174.434	-122.191	25.851
1033	36.500	98.725	67.805	31.940	-162.034	-122.191	25.851
1071	36.500	100.044	68.927	33.326	-161.506	-120.731	24.636
1071	36.500	100.044	68.927	33.326	-162.811	-120.731	24.636
1100	36.500	101.019	69.760	34.385	-162.409	-119.597	23.761
1200	36.500	104.195	72.499	38.035	-161.023	-115.771	21.085
1300	36.500	107.116	75.051	41.685	-159.638	-112.056	18.838

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
999 K, γ - δ transition point of Ce; $\Delta H°$ = 0.715 kcal/mol.
1033 K, melting point of CeI_3; $\Delta H°$ = 12.400 kcal/mol.
1071 K, melting point of Ce; $\Delta H°$ = 1.305 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1033 K: $Cp° = 22.499 + 6.312\times10^{-3}T - 0.338\times10^{5}T^{-2}$

$H°- H°_{298} = 22.499\times10^{-3}T + 3.156\times10^{-6}T^{2} + 0.338\times10^{2}T^{-1} - 7.102$

1033-1300 K: $Cp° = 36.500$

$H°- H°_{298} = 36.500\times10^{-3}T - 5.765$

CeI_3(c,l) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -154.813 - 1.901\times10^{-3}T - 1.029\times10^{-6}T^2 + 51.000T^{-1}$

$\Delta Gf^\circ = -154.813 + 1.901\times10^{-3}T\ln T + 1.029\times10^{-6}T^2 + 25.500T^{-1} - 8.525\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -156.995 - 11.508\times10^{-3}T + 1.209\times10^{-6}T^2 + 51.000T^{-1}$

$\Delta Gf^\circ = -156.995 + 11.508\times10^{-3}T\ln T - 1.209\times10^{-6}T^2 + 25.500T^{-1} - 59.248\times10^{-3}T$

458.4-999 K: $\Delta Hf^\circ = -179.065 + 4.003\times10^{-3}T + 1.107\times10^{-6}T^2 + 28.050T^{-1}$

$\Delta Gf^\circ = -179.065 - 4.003\times10^{-3}T\ln T - 1.107\times10^{-6}T^2 + 14.025T^{-1} + 83.946\times10^{-3}T$

999-1033 K: $\Delta Hf^\circ = -177.805 + 0.098\times10^{-3}T + 3.054\times10^{-6}T^2 + 10.850T^{-1}$

$\Delta Gf^\circ = -177.805 - 0.098\times10^{-3}T\ln T - 3.054\times10^{-6}T^2 + 5.425T^{-1} + 57.668\times10^{-3}T$

1033-1071 K: $\Delta Hf^\circ = -176.468 + 14.098\times10^{-3}T - 0.102\times10^{-6}T^2 - 22.950T^{-1}$

$\Delta Gf^\circ = -176.468 - 14.098\times10^{-3}T\ln T + 0.102\times10^{-6}T^2 - 11.475T^{-1} + 150.299\times10^{-3}T$

1071-1300 K: $\Delta Hf^\circ = -177.751 + 14.078\times10^{-3}T - 0.102\times10^{-6}T^2 - 22.950T^{-1}$

$\Delta Gf^\circ = -177.751 - 14.078\times10^{-3}T\ln T + 0.102\times10^{-6}T^2 - 11.475T^{-1} + 151.358\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (207). Enthalpy of fusion and heat capacity of liquid from Dworkin (66). All other data estimated.

$CeI_3(g)$

Cerium Triiodide (ideal gas)

[Formation: $Ce(c,l) + 1.5I_2(c,l,g) = CeI_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.496	102.111	102.111	0	-88.900	-101.802	74.622
300	19.501	102.232	102.112	.036	-88.912	-101.882	74.220
386.8	19.681	107.211	102.720	1.737	-89.594	-105.549	59.637
386.8	19.681	107.211	102.720	1.737	-95.158	-105.549	59.637
400	19.708	107.872	102.880	1.997	-95.369	-105.901	57.861
458.4	19.820	110.565	103.691	3.151	-96.303	-107.372	51.191
458.4	19.820	110.565	103.691	3.151	-111.335	-107.372	51.191
500	19.899	112.290	104.336	3.977	-111.359	-107.009	46.773
600	20.114	115.936	105.973	5.978	-111.431	-106.130	38.657
700	20.334	119.053	107.624	8.000	-111.521	-105.244	32.858
800	20.533	121.782	109.227	10.044	-111.632	-104.333	28.502
900	20.696	124.210	110.759	12.106	-111.769	-103.415	25.112
999	20.815	126.376	112.201	14.161	-111.930	-102.490	22.421
999	20.815	126.376	112.201	14.161	-112.645	-102.490	22.421
1000	20.816	126.397	112.215	14.182	-112.647	-102.482	22.397
1071	20.872	127.827	113.204	15.661	-112.771	-101.753	20.764
1071	20.872	127.827	113.204	15.661	-114.076	-101.753	20.764
1100	20.895	128.385	113.597	16.267	-114.127	-101.418	20.150
1200	20.939	130.205	114.906	18.359	-114.299	-100.259	18.259
1300	20.956	131.882	116.148	20.454	-114.468	-99.083	16.657
1400	20.950	133.435	117.328	22.550	-114.642	-97.889	15.281
1500	20.930	134.880	118.451	24.644	-114.818	-96.691	14.088
1600	20.898	136.230	119.521	26.735	-114.999	-95.477	13.041
1700	20.860	137.496	120.541	28.823	-115.186	-94.246	12.116
1800	20.818	138.687	121.516	30.907	-115.379	-93.018	11.294
1900	20.774	139.811	122.449	32.987	-115.578	-91.763	10.555
2000	20.730	140.876	123.345	35.062	-115.784	-90.510	9.890

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
999 K, γ - δ transition point of Ce; $\Delta H°$ = 0.715 kcal/mol.
1071 K, melting point of Ce; $\Delta H°$ = 1.305 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.938 + 0.714\times10^{-3}T - 0.582\times10^{5}T^{-2}$

$H°- H°_{298} = 19.938\times10^{-3}T + 0.357\times10^{-6}T^{2} + 0.582\times10^{2}T^{-1} - 6.171$

$CeI_3(g)$ - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -87.482 - 4.463\times10^{-3}T - 3.828\times10^{-6}T^2 + 75.400T^{-1}$

$\Delta Gf^\circ = -87.482 + 4.463\times10^{-3}T\ln T + 3.828\times10^{-6}T^2 + 37.700T^{-1} - 75.021\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -89.665 - 14.069\times10^{-3}T - 1.590\times10^{-6}T^2 + 75.400T^{-1}$

$\Delta Gf^\circ = -89.665 + 14.069\times10^{-3}T\ln T + 1.590\times10^{-6}T^2 + 37.700T^{-1} - 125.744\times10^{-3}T$

458.4-999 K: $\Delta Hf^\circ = -111.735 + 1.441\times10^{-3}T - 1.692\times10^{-6}T^2 + 52.450T^{-1}$

$\Delta Gf^\circ = -111.735 - 1.441\times10^{-3}T\ln T + 1.692\times10^{-6}T^2 + 26.225T^{-1} + 17.451\times10^{-3}T$

999-1071 K: $\Delta Hf^\circ = -110.474 - 2.464\times10^{-3}T + 0.255\times10^{-6}T^2 + 35.250T^{-1}$

$\Delta Gf^\circ = -110.474 + 2.464\times10^{-3}T\ln T - 0.255\times10^{-6}T^2 + 17.625T^{-1} - 8.828\times10^{-3}T$

1071-2000 K: $\Delta Hf^\circ = -111.758 - 2.484\times10^{-3}T + 0.255\times10^{-6}T^2 + 35.250T^{-1}$

$\Delta Gf^\circ = -111.758 + 2.484\times10^{-3}T\ln T - 0.255\times10^{-6}T^2 + 17.625T^{-1} - 7.769\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

ClF(g)

Chlorine Monofluoride (ideal gas)

[Formation: $0.5Cl_2(g) + 0.5F_2(g) = ClF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.668	52.062	52.062	0	-12.020	-12.376	9.072
300	7.676	52.110	52.063	.014	-12.021	-12.379	9.018
400	8.067	54.375	52.370	.802	-12.032	-12.497	6.828
500	8.333	56.205	52.959	1.623	-12.040	-12.612	5.512
600	8.513	57.742	53.632	2.466	-12.046	-12.726	4.635
700	8.638	59.064	54.315	3.324	-12.051	-12.838	4.008
800	8.729	60.224	54.983	4.193	-12.056	-12.951	3.538
900	8.797	61.256	55.624	5.069	-12.061	-13.062	3.172
1000	8.850	62.186	56.234	5.952	-12.065	-13.174	2.879
1100	8.893	63.031	56.814	6.839	-12.069	-13.284	2.639
1200	8.929	63.807	57.365	7.730	-12.074	-13.395	2.440
1300	8.960	64.523	57.888	8.625	-12.077	-13.504	2.270
1400	8.986	65.188	58.387	9.522	-12.082	-13.615	2.125
1500	9.010	65.808	58.860	10.422	-12.087	-13.723	1.999
1600	9.032	66.391	59.313	11.324	-12.092	-13.833	1.889
1700	9.052	66.939	59.746	12.228	-12.096	-13.941	1.792
1800	9.072	67.457	60.160	13.134	-12.102	-14.050	1.706
1900	9.092	67.948	60.557	14.042	-12.106	-14.157	1.628
2000	9.114	68.415	60.938	14.953	-12.111	-14.265	1.559

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.569 + 0.322\times10^{-3}T - 0.886\times10^{5}T^{-2}$

$H°- H°_{298} = 8.569\times10^{-3}T + 0.161\times10^{-6}T^{2} + 0.886\times10^{2}T^{-1} - 2.866$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -12.007 - 0.099\times10^{-3}T + 0.030\times10^{-6}T^{2} + 4.200T^{-1}$

$\Delta Gf° = -12.007 + 0.099\times10^{-3}T\ln T - 0.030\times10^{-6}T^{2} + 2.100T^{-1} - 1.814\times10^{-3}T$

Source: Data from Chase (24).

$ClF_3(g)$

Chlorine Trifluoride (ideal gas)

[Formation: $0.5Cl_2(g) + 1.5F_2(g) = ClF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	15.260	67.279	67.279	0	-37.970	-28.420	20.832
300	15.298	67.374	67.281	.028	-37.971	-28.362	20.661
400	16.875	72.012	67.902	1.644	-37.923	-25.163	13.748
500	17.798	75.885	69.121	3.382	-37.818	-21.983	9.609
600	18.366	79.184	70.531	5.192	-37.687	-18.829	6.858
700	18.734	82.045	71.976	7.048	-37.542	-15.698	4.901
800	18.984	84.564	73.395	8.935	-37.391	-12.589	3.439
900	19.162	86.811	74.763	10.843	-37.235	-9.496	2.306
1000	19.291	88.837	76.071	12.766	-37.079	-6.424	1.404
1100	19.389	90.680	77.316	14.700	-36.922	-3.365	.669
1200	19.464	92.370	78.501	16.643	-36.766	-.321	.058
1300	19.523	93.931	79.629	18.592	-36.610	2.710	-.456
1400	19.570	95.379	80.703	20.547	-36.457	5.728	-.894
1500	19.608	96.731	81.727	22.506	-36.306	8.735	-1.273
1600	19.640	97.997	82.705	24.468	-36.157	11.734	-1.603
1700	19.666	99.189	83.640	26.434	-36.007	14.724	-1.893
1800	19.688	100.314	84.535	28.402	-35.863	17.703	-2.149
1900	19.707	101.379	85.394	30.371	-35.719	20.676	-2.378
2000	19.723	102.390	86.218	32.343	-35.580	23.640	-2.583

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 18.982 + 0.534\times10^{-3}T - 3.450\times10^{5}T^{-2}$

$H°- H°_{298} = 18.982\times10^{-3}T + 0.267\times10^{-6}T^{2} + 3.450\times10^{2}T^{-1} - 6.840$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -39.042 + 1.806\times10^{-3}T - 0.038\times10^{-6}T^{2} + 160.100T^{-1}$

$\Delta Gf° = -39.042 - 1.806\times10^{-3}T\ln T + 0.038\times10^{-6}T^{2} + 80.050T^{-1} + 45.008\times10^{-3}T$

Source: Data from JANAF (60).

$ClF_5(g)$

Chlorine Pentafluoride (ideal gas)

[Formation: $0.5Cl_2(g) + 2.5F_2(g) = ClF_5(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	23.223	74.241	74.241	0	-57.000	-35.083	25.716
300	23.296	74.385	74.242	.043	-57.000	-34.947	25.459
400	26.295	81.539	75.197	2.537	-56.843	-27.614	15.087
500	28.013	87.608	77.088	5.260	-56.557	-20.337	8.889
600	29.058	92.815	79.287	8.117	-56.209	-13.127	4.781
700	29.732	97.348	81.549	11.059	-55.826	-5.976	1.866
800	30.188	101.350	83.779	14.057	-55.426	1.117	-.305
900	30.510	104.926	85.935	17.092	-55.014	8.162	-1.982
1000	30.746	108.153	87.997	20.156	-54.597	15.157	-3.313
1100	30.922	111.092	89.965	23.240	-54.176	22.114	-4.394
1200	31.058	113.789	91.840	26.339	-53.755	29.029	-5.287
1300	31.165	116.279	93.625	29.450	-53.332	35.913	-6.037
1400	31.250	118.592	95.327	32.571	-52.913	42.759	-6.675
1500	31.319	120.750	96.950	35.700	-52.494	49.579	-7.224
1600	31.376	122.773	98.501	38.835	-52.078	56.372	-7.700
1700	31.423	124.677	99.986	41.975	-51.663	63.140	-8.117
1800	31.463	126.474	101.408	45.119	-51.255	69.879	-8.484
1900	31.496	128.176	102.772	48.267	-50.845	76.600	-8.811
2000	31.525	129.792	104.083	51.418	-50.444	83.296	-9.102

*Enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 30.283 + 0.910\times10^{-3}T - 6.517\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 30.283\times10^{-3}T + 0.455\times10^{-6}T^2 + 6.517\times10^{2}T^{-1} - 11.255$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -59.598 + 4.599\times10^{-3}T - 0.024\times10^{-6}T^2 + 366.300T^{-1}$

$\Delta Gf^\circ = -59.598 - 4.599\times10^{-3}T\ln T + 0.024\times10^{-6}T^2 + 183.150T^{-1} + 106.363\times10^{-3}T$

Source: Data from JANAF (60) who estimated enthalpy of formation at 298 K.

CoCl(g)
Cobalt Monochloride (ideal gas)
[Formation: $Co(c,l) + 0.5Cl_2(g) = CoCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.398	58.692	58.692	0	46.100	38.686	-28.357
300	8.404	58.744	58.692	.016	46.097	38.641	-28.150
400	8.627	61.195	59.025	.868	45.920	36.175	-19.765
500	8.747	63.135	59.659	1.738	45.709	33.769	-14.760
600	8.819	64.736	60.376	2.616	45.460	31.403	-11.438
700	8.866	66.100	61.099	3.501	45.178	29.080	-9.079
700	8.866	66.100	61.099	3.501	45.070	29.080	-9.079
800	8.900	67.286	61.800	4.389	44.764	26.818	-7.326
900	8.925	68.336	62.469	5.280	44.409	24.594	-5.972
1000	8.945	69.277	63.103	6.174	44.002	22.404	-4.896
1100	8.961	70.130	63.704	7.069	43.532	20.274	-4.028
1200	8.976	70.911	64.273	7.966	42.988	18.180	-3.311
1300	8.989	71.630	64.812	8.864	42.344	16.135	-2.712
1394	9.001	72.257	65.292	9.710	41.599	14.259	-2.235
1400	9.002	72.296	65.322	9.764	41.557	14.142	-2.208
1500	9.015	72.918	65.808	10.665	41.015	12.198	-1.777
1600	9.028	73.500	66.271	11.567	40.533	10.292	-1.406
1700	9.043	74.048	66.713	12.470	40.074	8.415	-1.082
1768	9.055	74.403	67.001	13.085	39.765	7.149	-.884
1768	9.055	74.403	67.001	13.085	36.065	7.149	-.884
1800	9.060	74.565	67.134	13.375	35.840	6.629	-.805
1900	9.078	75.055	67.538	14.282	35.140	5.026	-.578
2000	9.100	75.522	67.927	15.191	34.440	3.458	-.378

Phase changes: 700 K, α - β transition point of Co; ΔH° = 0.108 kcal/mol.
1394 K, Curie temperature of Co; ΔH° = 0 kcal/mol.
1768 K, melting point of Co; ΔH° = 3.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.878 + 0.108\times10^{-3}T - 0.456\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.878\times10^{-3}T + 0.054\times10^{-6}T^2 + 0.456\times10^{2}T^{-1} - 2.805$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf^\circ = 46.418 - 0.537\times10^{-3}T - 1.767\times10^{-6}T^2 - 0.150T^{-1}$

$\Delta Gf^\circ = 46.418 + 0.537\times10^{-3}T\ln T + 1.767\times10^{-6}T2 - 0.075T^{-1} - 29.515\times10^{-3}T$

700-1394 K: $\Delta Hf^\circ = 39.886 + 7.950\times10^{-3}T - 5.405\times10^{-6}T^2 + 1586.250T^{-1}$

$\Delta Gf^\circ = 39.886 - 7.950\times10^{-3}T\ln T + 5.405\times10^{-6}T^2 + 793.125T^{-1} + 31.244\times10^{-3}T$

1394-1768 K: $\Delta Hf^\circ = 52.364 - 9.961\times10^{-3}T + 1.603\times10^{-6}T^2 + 11.450T^{-1}$

$\Delta Gf^\circ = 52.364 + 9.961\times10^{-3}T\ln T - 1.603\times10^{-6}T^2 + 5.725T^{-1} - 97.201\times10^{-3}T$

1768-2000 K: $\Delta Hf^\circ = 48.500 - 7.051\times10^{-3}T + 0.010\times10^{-6}T^2 + 11.450T^{-1}$

$\Delta Gf^\circ = 48.500 + 7.051\times10^{-3}T\ln T - 0.010\times10^{-6}T^2 + 5.725T^{-1} - 76.079\times10^{-3}T$

Source: Data from Chase (27) who estimated some molecular constants.

$CoCl_2(c,l)$

Cobalt Dichloride

[Formation: $Co(c) + Cl_2(g) = CoCl_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	18.760	26.115	26.115	0	-74.700	-64.457	47.248
300	18.779	26.231	26.115	.035	-74.691	-64.392	46.909
400	19.506	31.743	26.863	1.952	-74.218	-61.037	33.349
500	19.939	36.145	28.293	3.926	-73.752	-57.790	25.260
600	20.251	39.809	29.916	5.936	-73.303	-54.641	19.903
700	20.506	42.950	31.559	7.974	-72.871	-51.568	16.100
700	20.506	42.950	31.559	7.974	-72.979	-51.568	16.100
800	20.731	45.704	33.159	10.036	-72.555	-48.536	13.259
900	20.937	48.157	34.690	12.120	-72.161	-45.557	11.063
994	21.121	50.247	36.062	14.100	-71.822	-42.803	9.411
994*	24.000	60.810	36.062	24.600	-61.322	-42.803	9.411
1000	24.000	60.954	36.210	24.744	-61.285	-42.691	9.330
1100	24.000	63.242	38.566	27.144	-60.699	-40.854	8.117
1200	24.000	65.330	40.710	29.544	-60.190	-39.075	7.116
1300	24.000	67.251	42.679	31.944	-59.783	-37.336	6.277
1365	24.000	68.422	43.877	33.504	-59.602	-36.226	5.800

*Enthalpy of fusion and heat capacity of liquid estimated.

Phase changes: 700 K, α - β transition point of Co; ΔH° = 0.108 kcal/mol.
994 K, melting point of $CoCl_2$; ΔH° = 10.500 kcal/mol.
1365 K, calculated boiling point of $CoCl_2$ to monomer; ΔH° = 34.8 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-994 K: $Cp^\circ = 19.498 + 1.772\times10^{-3}T - 1.126\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.498\times10^{-3}T + 0.886\times10^{-6}T^2 + 1.126\times10^{2}T^{-1} - 6.270$

994-1365 K: $Cp^\circ = 24.000$

$H^\circ - H^\circ_{298} = 24.000\times10^{-3}T + 0.744$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf^\circ = -76.413 + 5.670\times10^{-3}T - 0.979\times10^{-6}T^2 + 32.700T^{-1}$

$\Delta Gf^\circ = -76.413 - 5.670\times10^{-3}T\ln T + 0.979\times10^{-6}T^2 + 16.350T^{-1} + 71.931\times10^{-3}T$

700-994 K: $\Delta Hf^\circ = -82.945 + 14.156\times10^{-3}T - 4.617\times10^{-6}T^2 + 1619.100T^{-1}$

$\Delta Gf^\circ = -82.945 - 14.156\times10^{-3}T\ln T + 4.617\times10^{-6}T^2 + 809.550T^{-1} + 132.689\times10^{-3}T$

994-1365 K: $\Delta Hf^\circ = -75.931 + 18.658\times10^{-3}T - 5.503\times10^{-6}T^2 + 1506.500T^{-1}$

$\Delta Gf^\circ = -75.931 - 18.658\times10^{-3}T\ln T + 5.503\times10^{-6}T^2 + 753.250T^{-1} + 155.881\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (253). Data for crystal from Chase (27). Temperature of fusion from Saeki (203). Enthalpy of fusion and heat capacity of liquid estimated.

$CoCl_2(g)$

Cobalt Dichloride (ideal gas)

[Formation: $Co(c,l) + Cl_2(g) = CoCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	14.250	71.316	71.316	0	-22.400	-25.634	18.790
300	14.256	71.404	71.317	.026	-22.400	-25.653	18.688
400	14.497	75.542	71.880	1.465	-22.405	-26.744	14.612
500	14.655	78.794	72.948	2.923	-22.455	-27.817	12.159
600	14.787	81.478	74.153	4.395	-22.544	-28.883	10.520
700	14.913	83.767	75.367	5.880	-22.665	-29.934	9.346
700	14.913	83.767	75.367	5.880	-22.773	-29.934	9.346
800	15.031	85.766	76.544	7.378	-22.913	-30.943	8.453
900	15.139	87.543	77.670	8.886	-23.095	-31.938	7.756
1000	15.233	89.143	78.738	10.405	-23.324	-32.919	7.194
1100	15.311	90.599	79.752	11.932	-23.611	-33.859	6.727
1200	15.374	91.934	80.712	13.467	-23.967	-34.777	6.334
1300	15.421	93.166	81.622	15.007	-24.420	-35.662	5.995
1394	15.453	94.245	82.438	16.458	-24.984	-36.465	5.717
1400	15.455	94.311	82.489	16.551	-25.015	-36.513	5.700
1500	15.479	95.378	83.313	18.097	-25.365	-37.327	5.439
1600	15.494	96.377	84.098	19.646	-25.654	-38.115	5.206
1700	15.502	97.317	84.849	21.196	-25.921	-38.885	4.999
1768	15.504	97.925	85.340	22.250	-26.100	-39.408	4.871
1768	15.504	97.925	85.340	22.250	-29.800	-39.408	4.871
1800	15.505	98.203	85.566	22.746	-29.965	-39.579	4.805
1900	15.505	99.041	86.253	24.297	-30.477	-40.097	4.612
2000	15.502	99.837	86.913	25.847	-30.994	-40.592	4.436

Phase changes: 700 K, α - β transition point of Co; ΔH° = 0.108 kcal/mol.
1394 K, Curie temperature of Co; ΔH° = 0 kcal/mol.
1768 K, melting point of Co; ΔH° = 3.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 14.514 + 0.674\times10^{-3}T - 0.414\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.514\times10^{-3}T + 0.337\times10^{-6}T^2 + 0.414\times10^{2}T^{-1} - 4.496$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf^\circ = -22.340 + 0.686\times10^{-3}T - 1.528\times10^{-6}T^2 - 38.500T^{-1}$

$\Delta Gf^\circ = -22.340 - 0.686\times10^{-3}T\ln T + 1.528\times10^{-6}T^2 - 19.250T^{-1} - 7.379\times10^{-3}T$

700-1394 K: $\Delta Hf^\circ = -28.871 + 9.172\times10^{-3}T - 5.166\times10^{-6}T^2 + 1547.900T^{-1}$

$\Delta Gf^\circ = -28.871 - 9.172\times10^{-3}T\ln T + 5.166\times10^{-6}T^2 + 773.950T^{-1} + 53.379\times10^{-3}T$

1394-1768 K: $\Delta Hf^\circ = -16.393 - 8.738\times10^{-3}T + 1.842\times10^{-6}T^2 - 26.900T^{-1}$

$\Delta Gf^\circ = -16.393 + 8.738\times10^{-3}T\ln T - 1.842\times10^{-6}T^2 - 13.450T^{-1} - 75.065\times10^{-3}T$

1768-2000 K: $\Delta Hf^\circ = -20.257 - 5.829\times10^{-3}T + 0.249\times10^{-6}T^2 - 26.900T^{-1}$

$\Delta Gf^\circ = -20.257 + 5.829\times10^{-3}T\ln T - 0.249\times10^{-6}T^2 - 13.450T^{-1} - 53.944\times10^{-3}T$

Source: Data from Chase (26).

$(CoCl_2)_2(g)$

Dimeric Cobalt Dichloride (ideal gas)

[Formation: $2Co(c,l) + 2Cl_2(g) = (CoCl_2)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	30.457	107.620	107.620	0	-83.800	-79.829	58.515
300	30.471	107.809	107.622	.056	-83.796	-79.803	58.135
400	31.014	116.659	108.824	3.134	-83.606	-78.514	42.897
500	31.309	123.614	111.112	6.251	-83.505	-77.243	33.762
600	31.515	129.341	113.686	9.393	-83.485	-75.994	27.680
700	31.684	134.212	116.279	12.553	-83.537	-74.748	23.337
700	31.684	134.212	116.279	12.553	-83.753	-74.748	23.337
800	31.831	138.453	118.792	15.729	-83.853	-73.451	20.066
900	31.959	142.210	121.189	18.919	-84.043	-72.141	17.518
1000	32.066	145.582	123.462	22.120	-84.338	-70.824	15.478
1100	32.155	148.643	125.615	25.331	-84.755	-69.440	13.796
1200	32.224	151.444	127.652	28.550	-85.318	-68.028	12.390
1300	32.278	154.025	129.582	31.776	-86.078	-66.564	11.190
1394	32.315	156.280	131.308	34.811	-87.074	-65.135	10.212
1400	32.317	156.419	131.415	35.005	-87.127	-65.039	10.153
1500	32.344	158.650	133.157	38.239	-87.685	-63.451	9.245
1600	32.362	160.738	134.817	41.474	-88.126	-61.822	8.444
1700	32.373	162.700	136.399	44.711	-88.523	-60.164	7.734
1768	32.376	163.970	137.436	46.912	-88.789	-59.040	7.298
1768	32.376	163.970	137.436	46.912	-96.189	-59.040	7.298
1800	32.378	164.551	137.913	47.948	-96.474	-58.363	7.086
1900	32.380	166.301	139.361	51.186	-97.362	-56.218	6.466
2000	32.378	167.962	140.750	54.424	-98.258	-54.030	5.904

Phase changes: 700 K, α - β transition point of Co; $\Delta H°$ = 0.108 kcal/mol.
1394 K, Curie temperature of Co; $\Delta H°$ = 0 kcal/mol.
1768 K, melting point of Co; $\Delta H°$ = 3.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 31.423 + 0.664\times10^{-3}T - 1.034\times10^{5}T^{-2}$

$H°- H°_{298} = 31.423\times10^{-3}T + 0.332\times10^{-6}T^2 + 1.034\times10^{2}T^{-1} - 9.745$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf° = -84.432 + 3.767\times10^{-3}T - 3.398\times10^{-6}T^2 - 56.400T^{-1}$

$\Delta Gf° = -84.432 - 3.767\times10^{-3}T\ln T + 3.398\times10^{-6}T^2 - 28.200T^{-1} + 36.206\times10^{-3}T$

700-1394 K: $\Delta Hf° = -97.496 + 20.739\times10^{-3}T - 10.674\times10^{-6}T^2 + 3116.400T^{-1}$

$\Delta Gf° = -97.496 - 20.739\times10^{-3}T\ln T + 10.674\times10^{-6}T^2 + 1558.200T^{-1} + 157.723\times10^{-3}T$

1394-1768 K: $\Delta Hf° = -72.540 - 15.081\times10^{-3}T + 3.342\times10^{-6}T^2 - 33.200T^{-1}$

$\Delta Gf° = -72.540 + 15.081\times10^{-3}T\ln T - 3.342\times10^{-6}T^2 - 16.600T^{-1} - 99.165\times10^{-3}T$

1768-2000 K: $\Delta Hf° = -80.267 - 9.263\times10^{-3}T + 0.156\times10^{-6}T^2 - 33.200T^{-1}$

$\Delta Gf° = -80.267 + 9.263\times10^{-3}T\ln T - 0.156\times10^{-6}T^2 - 16.600T^{-1} - 56.923\times10^{-3}T$

Source: Data from Chase (27) who estimated some molecular constants.

$CoCl_3(g)$
Cobalt Trichloride (ideal gas)
[Formation: $Co(c,l) + 1.5Cl_2(g) = CoCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	18.221	79.850	79.850	0	-39.100	-36.934	27.073
300	18.252	79.963	79.850	.034	-39.099	-36.919	26.895
400	19.375	85.389	80.581	1.923	-39.069	-36.202	19.780
500	19.851	89.772	81.996	3.888	-39.039	-35.483	15.510
600	20.041	93.411	83.604	5.884	-39.038	-34.773	12.666
700	20.109	96.506	85.232	7.892	-39.075	-34.062	10.634
700	20.109	96.506	85.232	7.892	-39.183	-34.062	10.634
800	20.127	99.193	86.813	9.904	-39.252	-33.325	9.104
900	20.129	101.563	88.322	11.917	-39.375	-32.577	7.911
1000	20.127	103.684	89.755	13.929	-39.557	-31.824	6.955
1100	20.127	105.602	91.109	15.942	-39.807	-31.032	6.165
1200	20.132	107.354	92.391	17.955	-40.135	-30.223	5.504
1300	20.140	108.966	93.605	19.969	-40.565	-29.384	4.940
1394	20.151	110.372	94.689	21.862	-41.112	-28.565	4.478
1400	20.152	110.459	94.757	21.983	-41.142	-28.510	4.451
1500	20.166	111.849	95.850	23.999	-41.475	-27.599	4.021
1600	20.181	113.151	96.891	26.016	-41.750	-26.666	3.642
1700	20.198	114.375	97.884	28.035	-42.003	-25.714	3.306
1768	20.210	115.167	98.533	29.409	-42.171	-25.067	3.099
1768	20.210	115.167	98.533	29.409	-45.871	-25.067	3.099
1800	20.215	115.530	98.832	30.056	-46.031	-24.687	2.997
1900	20.232	116.624	99.741	32.078	-46.528	-23.488	2.702
2000	20.249	117.662	100.611	34.102	-47.028	-22.263	2.433

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 700 K, α - β transition point of Co; ΔH° = 0.108 kcal/mol.
1394 K, Curie temperature of Co; ΔH° = 0 kcal/mol.
1768 K, melting point of Co; ΔH° = 3.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 20.940 - 0.478\times10^{-3}T - 2.291\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 20.940\times10^{-3}T - 0.239\times10^{-6}T^2 + 2.291\times10^{2}T^{-1} - 6.990$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf^\circ = -40.099 + 2.698\times10^{-3}T - 2.148\times10^{-6}T^2 + 115.050T^{-1}$

$\Delta Gf^\circ = -40.099 - 2.698\times10^{-3}T\ln T + 2.148\times10^{-6}T^2 + 57.525T^{-1} + 24.705\times10^{-3}T$

700-1394 K: $\Delta Hf^\circ = -46.631 + 11.185\times10^{-3}T - 5.786\times10^{-6}T^2 + 1701.450T^{-1}$

$\Delta Gf^\circ = -46.631 - 11.185\times10^{-3}T\ln T + 5.786\times10^{-6}T^2 + 850.725T^{-1} + 85.463\times10^{-3}T$

1394-1768 K: $\Delta Hf^\circ = -34.153 - 6.725\times10^{-3}T + 1.222\times10^{-6}T^2 + 126.650T^{-1}$

$\Delta Gf^\circ = -34.153 + 6.725\times10^{-3}T\ln T - 1.222\times10^{-6}T^2 + 63.325T^{-1} - 42.981\times10^{-3}T$

1768-2000 K: $\Delta Hf^\circ = -38.017 - 3.817\times10^{-3}T - 0.371\times10^{-6}T^2 + 126.650T^{-1}$

$\Delta Gf^\circ = -38.017 + 3.817\times10^{-3}T\ln T + 0.371\times10^{-6}T^2 + 63.325T^{-1} - 21.860\times10^{-3}T$

Source: Data from Chase (27) who estimated molecular constants.

$CoF_2(c,l)$
Cobalt Difluoride
[Formation: $Co(c) + F_2(g) = CoF_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	16.440	19.590	19.590	0	-160.700	-149.957	109.920
300	16.484	19.692	19.592	.030	-160.695	-149.890	109.193
400	18.074	24.683	20.260	1.769	-160.339	-146.344	79.958
500	18.886	28.811	21.569	3.621	-159.946	-142.885	62.454
600	19.394	32.302	23.075	5.536	-159.553	-139.511	50.816
700	19.760	35.321	24.614	7.495	-159.170	-136.204	42.524
700	19.760	35.321	24.614	7.495	-159.278	-136.204	42.524
800	20.049	37.979	26.122	9.486	-158.901	-132.931	36.314
900	20.294	40.355	27.574	11.503	-158.555	-129.706	31.497
1000	20.511	42.504	28.960	13.544	-158.248	-126.527	27.652
1100	20.710	44.469	30.283	15.605	-157.990	-123.361	24.509
1200	20.897	46.279	31.542	17.685	-157.792	-120.225	21.896
1300	21.076	47.958	32.740	19.784	-157.679	-117.101	19.686
1394	21.238	49.435	33.816	21.773	-157.702	-114.175	17.900
1400	21.248	49.526	33.883	21.900	-157.698	-113.988	17.794
1400*	24.000	59.312	33.883	35.600	-143.998	-113.988	17.794
1500	24.000	60.968	35.635	38.000	-143.491	-111.866	16.299

*Heat capacity of liquid estimated.

Phase changes: 700 K, α - β transition point of Co; ΔH° = 0.108 kcal/mol.
1394 K, Curie temperature of Co; ΔH° = 0 kcal/mol.
1400 K, melting point of CoF_2; ΔH° = 13.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1400 K: $Cp^\circ = 19.338 + 1.470\times10^{-3}T - 2.966\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 19.338\times10^{-3}T + 0.735\times10^{-6}T^2 + 2.966\times10^{2}T^{-1} - 6.826$

1400-1500 K: $Cp^\circ = 24.000$
$H^\circ - H^\circ_{298} = 24.000\times10^{-3}T + 2.000$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf^\circ = -162.949 + 5.829\times10^{-3}T - 1.216\times10^{-6}T^2 + 184.500T^{-1}$
$\Delta Gf^\circ = -162.949 - 5.829\times10^{-3}T\ln T + 1.216\times10^{-6}T^2 + 92.250T^{-1} + 75.386\times10^{-3}T$

700-1394 K: $\Delta Hf^\circ = -169.481 + 14.315\times10^{-3}T - 4.854\times10^{-6}T^2 + 1770.900T^{-1}$
$\Delta Gf^\circ = -169.481 - 14.315\times10^{-3}T\ln T + 4.854\times10^{-6}T^2 + 885.450T^{-1} + 136.144\times10^{-3}T$

1394-1400 K: $\Delta Hf^\circ = -157.002 - 3.595\times10^{-3}T + 2.154\times10^{-6}T^2 + 196.100T^{-1}$
$\Delta Gf^\circ = -157.002 + 3.595\times10^{-3}T\ln T - 2.154\times10^{-6}T^2 + 98.050T^{-1} + 7.700\times10^{-3}T$

1400-1500 K: $\Delta Hf^\circ = -148.177 + 1.067\times10^{-3}T + 1.419\times10^{-6}T^2 - 100.500T^{-1}$
$\Delta Gf^\circ = -148.177 - 1.067\times10^{-3}T\ln T - 1.419\times10^{-6}T^2 - 50.250T^{-1} + 34.215\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Chattopadhyay (28). Low-temperature heat capacities and entropy at 298 K from Catalano (22). High-temperature data based on Binford (16) except heat capacity of liquid which was estimated.

$CoF_2(g)$

Cobalt Difluoride (ideal gas)

[Formation: $Co(c,l) + F_2(g) = CoF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.239	66.421	66.421	0	-85.200	-88.419	64.812
300	12.252	66.497	66.421	.023	-85.202	-88.438	64.426
400	12.793	70.102	66.910	1.277	-85.331	-89.504	48.902
500	13.126	72.996	67.848	2.574	-85.493	-90.524	39.568
600	13.341	75.409	68.911	3.899	-85.690	-91.512	33.333
700	13.494	77.478	69.991	5.241	-85.924	-92.468	28.869
700	13.494	77.478	69.991	5.241	-86.032	-92.468	28.869
800	13.613	79.288	71.043	6.596	-86.291	-93.368	25.507
900	13.713	80.897	72.049	7.963	-86.595	-94.234	22.883
1000	13.803	82.347	73.009	9.338	-86.954	-95.076	20.779
1100	13.885	83.666	73.918	10.723	-87.372	-95.860	19.045
1200	13.960	84.877	74.781	12.115	-87.862	-96.612	17.595
1300	14.029	85.998	75.602	13.515	-88.448	-97.322	16.361
1394	14.089	86.979	76.336	14.836	-89.138	-97.949	15.356
1400	14.093	87.040	76.382	14.921	-89.177	-97.986	15.296
1500	14.150	88.014	77.125	16.333	-89.658	-98.602	14.366
1600	14.202	88.929	77.835	17.751	-90.076	-99.185	13.548
1700	14.250	89.791	78.513	19.173	-90.470	-99.742	12.823
1768	14.279	90.351	78.957	20.144	-90.733	-100.114	12.375
1768	14.279	90.351	78.957	20.144	-94.433	-100.114	12.375
1800	14.293	90.607	79.162	20.601	-94.637	-100.213	12.167
1900	14.331	91.381	79.785	22.032	-95.270	-100.506	11.561
2000	14.366	92.117	80.383	23.467	-95.904	-100.766	11.011

Phase changes: 700 K, α - β transition point of Co; ΔH° = 0.108 kcal/mol.
1394 K, Curie temperature of Co; ΔH° = 0 kcal/mol.
1768 K, melting point of Co; ΔH° = 3.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.243 + 0.640\times10^{-3}T - 1.062\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.243\times10^{-3}T + 0.320\times10^{-6}T^2 + 1.062\times10^{2}T^{-1} - 4.333$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf^\circ = -84.956 - 0.266\times10^{-3}T - 1.631\times10^{-6}T^2 - 5.900T^{-1}$

$\Delta Gf^\circ = -84.956 + 0.266\times10^{-3}T\ln T + 1.631\times10^{-6}T^2 - 2.950T^{-1} - 13.585\times10^{-3}T$

700-1394 K: $\Delta Hf^\circ = -91.488 + 8.220\times10^{-3}T - 5.269\times10^{-6}T^2 + 1580.500T^{-1}$

$\Delta Gf^\circ = -91.488 - 8.220\times10^{-3}T\ln T + 5.269\times10^{-6}T^2 + 790.250T^{-1} + 47.173\times10^{-3}T$

1394-1768 K: $\Delta Hf^\circ = -79.010 - 9.690\times10^{-3}T + 1.739\times10^{-6}T^2 + 5.700T^{-1}$

$\Delta Gf^\circ = -79.010 + 9.690\times10^{-3}T\ln T - 1.739\times10^{-6}T^2 + 2.850T^{-1} - 81.271\times10^{-3}T$

1768-2000 K: $\Delta Hf^\circ = -82.873 - 6.781\times10^{-3}T + 0.146\times10^{-6}T^2 + 5.700T^{-1}$

$\Delta Gf^\circ = -82.873 + 6.781\times10^{-3}T\ln T - 0.146\times10^{-6}T^2 + 2.850T^{-1} - 60.150\times10^{-3}T$

Source: Data from JANAF (60) who estimated most molecular constants.

$CoF_3(c)$
Cobalt Trifluoride
[Formation: $Co(c) + 1.5F_2(g) = CoF_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	21.940	22.600	22.600	0	-188.900	-171.833	125.955
300	22.101	22.736	22.600	.041	-188.891	-171.726	125.101
400	23.296	29.274	23.484	2.316	-188.383	-166.085	90.744
500	23.829	34.536	25.186	4.675	-187.885	-160.564	70.181
600	24.009	38.896	27.118	7.067	-187.430	-155.144	56.510
700	24.192	42.611	29.072	9.477	-187.020	-149.798	46.768
700	24.192	42.611	29.072	9.477	-187.128	-149.798	46.768
800	24.374	45.853	30.972	11.905	-186.745	-144.489	39.472
900	24.579	48.735	32.787	14.353	-186.404	-139.227	33.809
1000	24.825	51.338	34.515	16.823	-186.108	-134.014	29.288
1100	25.102	53.716	36.153	19.319	-185.858	-128.808	25.591
1200	25.394	55.913	37.710	21.843	-185.661	-123.634	22.517
1300	25.714	57.958	39.190	24.399	-185.539	-118.472	19.917
1394	26.017	59.764	40.518	26.830	-185.543	-113.634	17.815
1400	26.036	59.876	40.600	26.986	-185.537	-113.324	17.690

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 700 K, α - β transition point of Co; ΔH° = 0.108 kcal/mol.
1394 K, Curie temperature of Co; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1400 K: $Cp^\circ = 23.968 + 1.166\times10^{-3}T - 2.111\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 23.968\times10^{-3}T + 0.583\times10^{-6}T^2 + 2.111\times10^{2}T^{-1} - 7.906$

Formation equations (kcal/mol):

298.15-700 K: $\Delta Hf^\circ = -190.784 + 6.205\times10^{-3}T - 1.455\times10^{-6}T^2 + 48.750T^{-1}$

$\Delta Gf^\circ = -190.784 - 6.205\times10^{-3}T\ln T + 1.455\times10^{-6}T^2 + 24.375T^{-1} + 98.210\times10^{-3}T$

700-1394 K: $\Delta Hf^\circ = -197.316 + 14.691\times10^{-3}T - 5.093\times10^{-6}T^2 + 1635.150T^{-1}$

$\Delta Gf^\circ = -197.316 - 14.691\times10^{-3}T\ln T + 5.093\times10^{-6}T^2 + 817.575T^{-1} + 158.968\times10^{-3}T$

1394-1400 K: $\Delta Hf^\circ = -184.838 - 3.219\times10^{-3}T + 1.915\times10^{-6}T^2 + 60.350T^{-1}$

$\Delta Gf^\circ = -184.838 + 3.219\times10^{-3}T\ln T - 1.915\times10^{-6}T^2 + 30.175T^{-1} + 30.524\times10^{-3}T$

Source: Data from Chase (25) who estimated all except enthalpy of formation at 298 K.

$CrBr_3(c)$
Chromium Tribromide
[Formation: $Cr(c) + 1.5Br_2(l,g) = CrBr_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	23.050	38.162	38.162	0	-103.400	-96.824	70.973
300*	23.070	38.305	38.162	.043	-103.417	-96.783	70.506
311.5	23.159	39.174	38.183	.309	-103.529	-96.526	67.722
332.6	23.321	40.698	38.295	.799	-103.766	-96.045	63.110
332.6	23.321	40.698	38.295	.799	-114.364	-96.045	63.110
400	23.840	45.057	39.077	2.392	-114.012	-92.376	50.471
500	24.320	50.433	40.829	4.802	-113.547	-87.020	38.036
600	24.680	54.900	42.813	7.252	-113.087	-81.757	29.780
700	24.970	58.726	44.819	9.735	-112.630	-76.570	23.906
800	25.220	62.077	46.771	12.245	-112.174	-71.449	19.519
900	25.470	65.063	48.642	14.779	-111.719	-66.388	16.121
1000	25.700	67.758	50.420	17.338	-111.262	-61.377	13.414
1100	25.940	70.219	52.110	19.920	-110.819	-56.409	11.207

*Data above 298 K estimated.

Phase changes: 311.5 K, second order transition point of Cr; $\Delta H°$ = 0 kcal/mol.
322.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp° = 23.743 + 2.082\times10^{-3}T - 1.168\times10^{5}T^{-2}$

$H°- H°_{298} = 23.743\times10^{-3}T + 1.041\times10^{-6}T^{2} + 1.168\times10^{2}T^{-1} - 7.563$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf° = -102.473 - 0.585\times10^{-3}T - 12.876\times10^{-6}T^{2} + 116.800T^{-1}$

$\Delta Gf° = -102.473 + 0.585\times10^{-3}T\ln T + 12.876\times10^{-6}T^{2} + 58.400T^{-1} + 11.114\times10^{-3}T$

311.5-332.6 K: $\Delta Hf° = -101.475 - 7.753\times10^{-3}T - 0.600\times10^{-6}T^{2} + 130.400T^{-1}$

$\Delta Gf° = -101.475 + 7.753\times10^{-3}T\ln T + 0.600\times10^{-6}T^{2} + 65.200T^{-1} - 29.484\times10^{-3}T$

332.6-1100 K: $\Delta Hf° = -116.475 + 5.989\times10^{-3}T - 0.833\times10^{-6}T^{2} + 83.300T^{-1}$

$\Delta Gf° = -116.475 - 5.989\times10^{-3}T\ln T + 0.833\times10^{-6}T^{2} + 41.650T^{-1} + 95.549\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Shchukarev (209). Low-temperature heat capacities and entropy at 298 K from Jennings (108). High-temperature data estimated.

$CrBr_4$(g)

Chromium Tetrabromide (ideal gas)

[Formation: $Cr(c) + 2Br_2(l,g) = CrBr_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	24.218	99.739	99.739	0	-61.800	-68.160	49.962
300	24.237	99.901	99.741	.048	-61.828	-68.200	49.683
311.5	24.312	100.814	99.764	.327	-62.031	-68.440	48.017
332.6	24.448	102.412	99.882	.842	-62.434	-68.862	45.248
332.6	24.448	102.412	99.882	.842	-76.564	-68.862	45.248
400	24.885	106.974	100.701	2.509	-76.432	-67.324	36.784
500	25.211	112.566	102.536	5.015	-76.312	-65.061	28.438
600	25.395	117.180	104.603	7.546	-76.215	-62.818	22.881
700	25.509	121.104	106.687	10.092	-76.142	-60.591	18.917
800	25.584	124.515	108.706	12.647	-76.089	-58.371	15.946
900	25.637	127.532	110.634	15.208	-76.056	-56.161	13.637
1000	25.674	130.235	112.461	17.774	-76.042	-53.953	11.791
1100	25.702	132.683	114.190	20.342	-76.064	-51.742	10.280
1200	25.723	134.921	115.826	22.914	-76.122	-49.524	9.019
1300	25.740	136.980	117.375	25.487	-76.230	-47.313	7.954

*$CrBr_4$ stable only in presence of Br_2(g).

Phase changes: 311.5 K, second order transition point of Cr; $\Delta H° = 0$ kcal/mol.
332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $Cp° = 25.727 + 0.082\times10^{-3}T - 1.363\times10^{5}T^{-2}$

$H°- H°_{298} = 25.727\times10^{-3}T + 0.041\times10^{-6}T^2 + 1.363\times10^{2}T^{-1} - 8.131$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf° = -58.748 - 7.647\times10^{-3}T - 13.826\times10^{-6}T^2 + 136.300T^{-1}$

$\Delta Gf° = -58.748 + 7.647\times10^{-3}T\ln T + 13.826\times10^{-6}T^2 + 68.150T^{-1} - 80.025\times10^{-3}T$

311.5-332.6 K: $\Delta Hf° = -57.750 - 14.814\times10^{-3}T - 1.550\times10^{-6}T^2 + 149.900T^{-1}$

$\Delta Gf° = -57.750 + 14.814\times10^{-3}T\ln T + 1.550\times10^{-6}T^2 + 74.950T^{-1} - 120.623\times10^{-3}T$

332.6-1300 K: $\Delta Hf° = -77.751 + 3.508\times10^{-3}T - 1.860\times10^{-6}T^2 + 87.100T^{-1}$

$\Delta Gf° = -77.751 - 3.508\times10^{-3}T\ln T + 1.860\times10^{-6}T^2 + 43.550T^{-1} + 46.087\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Shchukarev (209). Other data from Cuoni (53).

$CrCl_2(c,1)$

Chromium Dichloride

[Formation: $Cr(c) + Cl_2(g) = CrCl_2(c,1)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	17.010	27.560	27.560	0	-94.500	-85.144	62.411
300*	17.030	27.665	27.562	.031	-94.494	-85.088	61.985
311.5	17.135	28.308	27.577	.227	-94.458	-84.727	59.444
400	17.940	32.698	28.241	1.783	-94.153	-82.002	44.803
500	18.570	36.773	29.553	3.610	-93.801	-79.003	34.532
600	19.060	40.203	31.050	5.492	-93.446	-76.076	27.710
700	19.460	43.171	32.574	7.418	-93.085	-73.208	22.856
800	19.810	45.792	34.064	9.382	-92.719	-70.394	19.231
900	20.130	48.144	35.501	11.379	-92.342	-67.625	16.421
1000	20.450	50.282	36.874	13.408	-91.959	-64.903	14.184
1088	20.730	52.018	38.029	15.220	-91.626	-62.534	12.561
1088	24.000	59.095	38.029	22.920	-83.926	-62.534	12.561
1100	24.000	59.359	38.261	23.208	-83.842	-62.300	12.378
1200	24.000	61.447	40.107	25.608	-83.166	-60.367	10.994
1300	24.000	63.368	41.823	28.008	-82.539	-58.502	9.835

*Data above 298 K except temperature and enthalpy of fusion estimated.

Phase changes: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.
1088 K, melting point of $CrCl_2$; ΔH° = 7.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1088 K: $C_p^\circ = 17.506 + 3.106\times10^{-3}T - 1.264\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 17.506\times10^{-3}T + 1.553\times10^{-6}T^2 + 1.264\times10^{2}T^{-1} - 5.781$

1088-1300 K: $C_p^\circ = 24.000$

$H^\circ - H^\circ_{298} = 24.000\times10^{-3}T - 3.192$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf^\circ = -96.999 + 11.487\times10^{-3}T - 12.602\times10^{-6}T^2 + 58.100T^{-1}$

$\Delta Gf^\circ = -96.999 - 11.487\times10^{-3}T\ln T + 12.602\times10^{-6}T^2 + 29.050T^{-1} + 101.128\times10^{-3}T$

311.5-1088 K: $\Delta Hf^\circ = -96.002 + 4.320\times10^{-3}T - 0.326\times10^{-6}T^2 + 71.700T^{-1}$

$\Delta Gf^\circ = -96.002 - 4.320\times10^{-3}T\ln T + 0.326\times10^{-6}T^2 + 35.850T^{-1} + 60.530\times10^{-3}T$

1088-1300 K: $\Delta Hf^\circ = -93.413 + 10.814\times10^{-3}T - 1.879\times10^{-6}T^2 - 54.700T^{-1}$

$\Delta Gf^\circ = -93.413 - 10.814\times10^{-3}T\ln T + 1.879\times10^{-6}T^2 - 27.350T^{-1} + 101.921\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (253). Low-temperature heat capacities and entropy at 298 K from Stout (208). Temperature and enthalpy of fusion from Maier (151). All other data estimated.

$CrCl_3(c)$

Chromium Trichloride

[Formation: $Cr(c) + 1.5Cl_2(g) = CrCl_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	21.940	29.380	29.380	0	-133.000	-116.242	85.207
300*	21.970	29.516	29.380	.041	-132.992	-116.139	84.606
311.5	22.134	30.346	29.400	.295	-132.945	-115.494	81.030
400	23.400	36.050	30.262	2.315	-132.544	-110.589	60.422
500	24.340	41.379	31.969	4.705	-132.055	-105.153	45.962
600	25.010	45.879	33.922	7.174	-131.548	-99.819	36.359
700	25.540	49.776	35.915	9.703	-131.022	-94.571	29.526
800	25.980	53.216	37.866	12.280	-130.486	-89.402	24.423
900	26.360	56.299	39.746	14.898	-129.934	-84.298	20.470
1000	26.710	59.094	41.543	17.551	-129.374	-79.261	17.322
1100	27.030	61.655	43.257	20.238	-128.818	-74.275	14.757
1200	27.340	64.020	44.890	22.956	-128.274	-69.337	12.628

*Data above 298 K estimated.

Phase changes: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.
1280 ±10 K, sublimation point of $CrCl_3$; ΔH° (sublimation, 298 K) = 56.5 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp^\circ = 23.621 + 3.336\times10^{-3}T - 2.378\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 23.621\times10^{-3}T + 1.668\times10^{-6}T^2 + 2.378\times10^{2}T^{-1} - 7.988$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf^\circ = -136.272 + 13.189\times10^{-3}T - 12.531\times10^{-6}T^2 + 135.350T^{-1}$

$\Delta Gf^\circ = -136.272 - 13.189\times10^{-3}T\ln T + 12.531\times10^{-6}T^2 + 67.675T^{-1} + 137.825\times10^{-3}T$

311.5-1200 K: $\Delta Hf^\circ = -135.274 + 6.021\times10^{-3}T - 0.255\times10^{-6}T^2 + 148.950T^{-1}$

$\Delta Gf^\circ = -135.274 - 6.021\times10^{-3}T\ln T + 0.255\times10^{-6}T^2 + 74.475T^{-1} + 97.228\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (253). Low-temperature heat capacities and entropy at 298 K from Hansen (97). Data 300-1200 K estimated. Sublimation data from Oppermann (175).

$CrCl_4(g)$

Chromium Tetrachloride (ideal gas)

[Formation: $Cr(c) + 2Cl_2(g) = CrCl_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	22.973	87.068	87.068	0	-102.000	-94.498	69.268
300	23.003	87.222	87.069	.046	-101.994	-94.453	68.808
311.5	23.128	88.090	87.090	.311	-101.983	-94.163	66.065
400	24.093	94.006	87.988	2.407	-101.874	-91.956	50.242
500	24.670	99.451	89.755	4.848	-101.761	-89.487	39.114
600	25.006	103.981	91.759	7.333	-101.672	-87.041	31.704
700	25.217	107.853	93.789	9.845	-101.603	-84.608	26.415
800	25.358	111.229	95.761	12.374	-101.558	-82.184	22.451
900	25.456	114.222	97.649	14.916	-101.526	-79.762	19.369
1000	25.527	116.908	99.443	17.465	-101.517	-77.349	16.904
1100	25.579	119.344	101.144	20.020	-101.542	-74.931	14.887
1200	25.620	121.571	102.754	22.580	-101.606	-72.505	13.205
1300	25.652	123.623	104.281	25.144	-101.717	-70.084	11.782

*$CrCl_4$ stable only in presence of $Cl_2(g)$.

Phase change: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $Cp^\circ = 25.438 + 0.314\times10^{-3}T - 2.274\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.438\times10^{-3}T + 0.157\times10^{-6}T^2 + 2.274\times10^{2}T^{-1} - 8.361$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf^\circ = -104.210 + 10.592\times10^{-3}T - 14.086\times10^{-6}T^2 + 90.800T^{-1}$

$\Delta Gf^\circ = -104.210 - 10.592\times10^{-3}T\ln T + 14.086\times10^{-6}T^2 + 45.400T^{-1} + 88.214\times10^{-3}T$

311.5-1300 K: $\Delta Hf^\circ = -103.213 + 3.425\times10^{-3}T - 1.810\times10^{-6}T^2 + 104.400T^{-1}$

$\Delta Gf^\circ = -103.213 - 3.425\times10^{-3}T\ln T + 1.810\times10^{-6}T^2 + 52.200T^{-1} + 47.617\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (253). Other data from Cuoni (53).

$CrF_2(c)$
Chromium Difluoride
[Formation: $Cr(c) + F_2(g) = CrF_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	15.480	20.762	20.762	0	-186.000	-176.062	129.056
300*	15.510	20.858	20.762	.029	-185.995	-176.002	128.215
311.5	15.649	21.444	20.776	.208	-185.969	-175.619	123.213
400	16.720	25.504	21.386	1.647	-185.727	-172.709	94.362
500	17.430	29.316	22.604	3.356	-185.444	-169.485	74.081
600	17.970	32.543	23.998	5.127	-185.161	-166.320	60.581
700	18.460	35.350	25.424	6.948	-184.875	-163.202	50.953
800	18.950	37.847	26.823	8.819	-184.578	-160.126	43.744
900	19.450	40.107	28.175	10.739	-184.259	-157.086	38.145
1000	19.940	42.182	29.474	12.708	-183.922	-154.089	33.676
1100	20.410	44.104	30.717	14.726	-183.576	-151.119	30.024
1200	20.840	45.899	31.908	16.789	-183.228	-148.181	26.987

*Data above 298 K estimated.

Phase changes: 298.15 K, ΔH° (sublimation) = 82.0 ±3.5 kcal/mol.
311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.
1167 ±6 K, melting point of CrF_2; ΔH° unknown.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp^\circ = 15.896 + 4.182\times10^{-3}T - 1.479\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 15.896\times10^{-3}T + 2.091\times10^{-6}T^2 + 1.479\times10^{2}T^{-1} - 5.421$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf^\circ = -188.119 + 10.196\times10^{-3}T - 12.150\times10^{-6}T^2 + 47.400T^{-1}$

$\Delta Gf^\circ = -188.119 - 10.196\times10^{-3}T\ln T + 12.150\times10^{-6}T^2 + 23.700T^{-1} + 94.641\times10^{-3}T$

311.5-1200 K: $\Delta Hf^\circ = -187.121 + 3.029\times10^{-3}T + 0.126\times10^{-6}T^2 + 61.000T^{-1}$

$\Delta Gf^\circ = -187.121 - 3.029\times10^{-3}T\ln T - 0.126\times10^{-6}T^2 + 30.500T^{-1} + 54.044\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (253). Low-temperature heat capacities and entropy at 298 K from Boo (17). Data above 298 K estimated. Temperature of fusion from Sturm (229). Sublimation data from Malkerova (153).

$CrF_3(c)$
Chromium Trifluoride
[Formation: $Cr(c) + 1.5F_2(g) = CrF_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.820	22.438	22.438	0	-280.400	-263.740	193.324
300*	18.870	22.555	22.438	.035	-280.396	-263.638	192.058
311.5	19.111	23.269	22.456	.253	-280.374	-262.996	184.517
400	20.970	28.298	23.208	2.036	-280.129	-258.089	141.011
500	22.180	33.119	24.721	4.199	-279.794	-252.614	110.416
600	22.910	37.231	26.471	6.456	-279.440	-247.211	90.045
700	23.400	40.802	28.271	8.772	-279.083	-241.867	75.513
800	23.800	43.953	30.037	11.133	-278.728	-236.576	64.629
900	24.150	46.777	31.743	13.531	-278.366	-231.326	56.173
1000	24.500	49.340	33.377	15.963	-278.006	-226.123	49.419
1100	24.840	51.691	34.936	18.431	-277.653	-220.949	43.898
1200	25.160	53.867	36.425	20.931	-277.314	-215.807	39.303

*Data above 298 K estimated.

Phase changes: 311.5 K, second order transition point of Cr; $\Delta H° = 0$ kcal/mol.
1680 ±20 K, melting point of CrF_3; $\Delta H°$ unknown.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 22.459 + 2.450\times10^{-3}T - 3.884\times10^{5}T^{-2}$

$H°- H°_{298} = 22.459\times10^{-3}T + 1.225\times10^{-6}T^2 + 3.884\times10^{2}T^{-1} - 8.108$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta Hf° = -283.761 + 12.505\times10^{-3}T - 13.103\times10^{-6}T^2 + 237.650T^{-1}$

$\Delta Gf° = -283.761 - 12.505\times10^{-3}T\ln T + 13.103\times10^{-6}T^2 + 118.825T^{-1} + 133.153\times10^{-3}T$

311.5-1200 K: $\Delta Hf° = -282.763 + 5.338\times10^{-3}T - 0.827\times10^{-6}T^2 + 251.250T^{-1}$

$\Delta Gf° = -282.763 - 5.338\times10^{-3}T\ln T + 0.827\times10^{-6}T^2 + 125.625T^{-1} + 92.556\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Schaefer (205). Low-temperature heat capacities and entropy at 298 K from Hansen (97). Temperature of fusion from Sturm (29). Data above 298 K estimated.

CsBr(c,1)

Cesium Bromide

[Formation: $Cs(c,l,g) + 0.5Br_2(l,g) = CsBr(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.440	27.020	27.020	0	-96.990	-93.549	68.573
300	12.446	27.097	27.020	.023	-96.997	-93.528	68.134
301.55	12.451	27.161	27.021	.042	-97.004	-93.510	67.771
301.55	12.451	27.161	27.021	.042	-97.504	-93.510	67.771
332.6	12.545	28.386	27.092	.430	-97.636	-93.092	61.170
332.6	12.545	28.386	27.092	.430	-101.168	-93.092	61.170
400	12.751	30.721	27.514	1.283	-101.120	-91.462	49.972
500	13.133	33.605	28.451	2.577	-101.016	-89.058	38.927
600	13.682	36.045	29.518	3.916	-100.863	-86.679	31.573
700	14.425	38.207	30.608	5.319	-100.647	-84.332	26.329
800	15.372	40.193	31.684	6.807	-100.346	-82.022	22.407
900	16.530	42.068	32.734	8.401	-99.941	-79.753	19.366
909	16.645	42.233	32.827	8.550	-99.899	-79.552	19.126
909	18.600	48.438	32.827	14.190	-94.259	-79.552	19.126
952	18.600	49.298	33.552	14.990	-93.971	-78.875	18.107
952	18.600	49.298	33.552	14.990	-110.169	-78.875	18.107
1000	18.600	50.212	34.329	15.883	-109.730	-77.307	16.895
1100	18.600	51.985	35.855	17.743	-108.818	-74.109	14.724
1200	18.600	53.604	37.268	19.603	-107.906	-70.993	12.930
1300	18.600	55.092	38.582	21.463	-106.995	-67.953	11.424
1400	18.600	56.471	39.812	23.323	-106.086	-64.985	10.144

Phase changes: 301.55 K, melting point of Cs; ΔH° = 0.500 kcal/mol.
332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
909 K, melting point of CsBr; ΔH° = 5.640 kcal/mol.
952 K, boiling point of Cs to ideal monatomic gas; ΔH° = 16.198 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-909 K: $Cp^\circ = 8.635 + 8.134\times10^{-3}T + 1.225\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.635\times10^{-3}T + 4.067\times10^{-6}T^2 - 1.225\times10^{2}T^{-1} - 2.525$

909-1400 K: $Cp^\circ = 18.600$

$H^\circ - H^\circ_{298} = 18.600\times10^{-3}T - 2.717$

CsBr(c,l) - Continued

Formation equations (kcal/mol):

298.15-301.55 K: $\Delta Hf^\circ = -95.208 - 3.546\times10^{-3}T - 3.530\times10^{-6}T^2 - 122.500T^{-1}$

$\Delta Gf^\circ = -95.208 + 3.546\times10^{-3}T\ln T + 3.530\times10^{-6}T^2 - 61.250T^{-1} - 15.008\times10^{-3}T$

301.55-332.6 K: $\Delta Hf^\circ = -95.351 - 7.543\times10^{-3}T + 4.002\times10^{-6}T^2 - 73.200T^{-1}$

$\Delta Gf^\circ = -95.351 + 7.543\times10^{-3}T\ln T - 4.002\times10^{-6}T^2 - 36.600T^{-1} - 35.351\times10^{-3}T$

332.6-909 K: $\Delta Hf^\circ = -100.351 - 2.963\times10^{-3}T + 3.924\times10^{-6}T^2 - 88.900T^{-1}$

$\Delta Gf^\circ = -100.351 + 2.963\times10^{-3}T\ln T - 3.924\times10^{-6}T^2 - 44.450T^{-1} + 6.326\times10^{-3}T$

909-952 K: $\Delta Hf^\circ = -100.544 + 7.002\times10^{-3}T - 0.143\times10^{-6}T^2 + 33.600T^{-1}$

$\Delta Gf^\circ = -100.544 - 7.002\times10^{-3}T\ln T + 0.143\times10^{-6}T^2 + 16.800T^{-1} + 70.652\times10^{-3}T$

952-1400 K: $\Delta Hf^\circ = -119.079 + 9.376\times10^{-3}T - 0.091\times10^{-6}T^2 + 63.200T^{-1}$

$\Delta Gf^\circ = -119.079 - 9.376\times10^{-3}T\ln T + 0.091\times10^{-6}T^2 + 31.600T^{-1} + 106.436\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (255). Low-temperature heat capacities from Sorai (221). High-temperature data for crystal based on Bibas (14). Heat capacity of liquid based on Murgulescu (162). Enthalpy of fusion from Dworkin (65).

CsCl(c,1)

Cesium Chloride

[Formation: $Cs(c,l,g) + 0.5Cl_2(g) = CsCl(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	12.540	24.180	24.180	0	-105.890	-99.082	72.628
300	12.550	24.258	24.181	.023	-105.888	-99.039	72.149
301.55	12.557	24.323	24.182	.042	-105.887	-99.004	71.753
301.55	12.557	24.323	24.182	.042	-106.387	-99.004	71.753
400	12.993	27.933	24.678	1.302	-106.286	-96.607	52.783
500	13.318	30.869	25.633	2.618	-106.146	-94.204	41.176
600	13.562	33.320	26.715	3.963	-105.978	-91.830	33.449
700	13.733	35.425	27.814	5.328	-105.791	-89.487	27.939
743	13.786	36.245	28.277	5.920	-105.707	-88.488	26.028
743	15.830	37.725	28.277	7.020	-104.607	-88.488	26.028
800	15.830	38.895	28.993	7.922	-104.381	-87.260	23.838
900	15.830	40.760	30.199	9.505	-103.982	-85.144	20.676
918	15.830	41.073	30.408	9.790	-103.910	-84.767	20.180
918	17.740	46.367	30.408	14.650	-99.050	-84.767	20.180
952	17.740	47.012	30.990	15.253	-98.851	-84.255	19.342
952	17.740	47.012	30.990	15.253	-115.049	-84.255	19.342
1000	17.740	47.885	31.780	16.105	-114.650	-82.712	18.076
1100	17.740	49.576	33.322	17.879	-113.821	-79.558	15.806
1200	17.740	51.119	34.742	19.653	-112.993	-76.478	13.928
1300	17.740	52.539	36.057	21.427	-112.167	-73.469	12.351
1400	17.740	53.854	37.282	23.201	-111.343	-70.523	11.009

Phase changes: 301.55 K, melting point of Cs; $\Delta H°$ = 0.500 kcal/mol.
743 K, α - β transition point of CsCl; $\Delta H°$ = 1.100 kcal/mol.
918 K, melting point of CsCl; $\Delta H°$ = 4.860 kcal.mol.
952 K, boiling point of Cs to ideal monatomic gas; $\Delta H°$ = 16.198 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-743 K: $Cp° = 12.625 + 1.788\times10^{-3}T - 0.549\times10^{5}T^{-2}$

$H°- H°_{298} = 12.625\times10^{-3}T + 0.894\times10^{-6}T^{2} + 0.549\times10^{2}T^{-1} - 4.028$

743-918 K: $Cp° = 15.830$

$H°- H°_{298} = 15.830\times10^{-3}T - 4.742$

918-1400 K: $Cp° = 17.740$

$H°- H°_{298} = 17.740\times10^{-3}T - 1.635$

CsCl(c,l) - Continued

Formation equations (kcal/mol):

298.15-301.55 K: $\Delta Hf^\circ = -106.869 + 5.076\times10^{-3}T - 6.797\times10^{-6}T^2 + 20.750T^{-1}$

$\Delta Gf^\circ = -106.869 - 5.076\times10^{-3}T\ln T + 6.797\times10^{-6}T^2 + 10.375T^{-1} + 52.892\times10^{-3}T$

301.55-743 K: $\Delta Hf^\circ = -107.012 + 1.079\times10^{-3}T + 0.735\times10^{-6}T^2 + 70.050T^{-1}$

$\Delta Gf^\circ = -107.012 - 1.079\times10^{-3}T\ln T - 0.735\times10^{-6}T^2 + 35.025T^{-1} + 32.548\times10^{-3}T$

743-918 K: $\Delta Hf^\circ = -107.726 + 4.283\times10^{-3}T - 0.159\times10^{-6}T^2 + 15.150T^{-1}$

$\Delta Gf^\circ = -107.726 - 4.283\times10^{-3}T\ln T + 0.159\times10^{-6}T^2 + 7.575T^{-1} + 54.082\times10^{-3}T$

918-952 K: $\Delta Hf^\circ = -104.619 + 6.194\times10^{-3}T - 0.159\times10^{-6}T^2 + 15.150T^{-1}$

$\Delta Gf^\circ = -104.619 - 6.194\times10^{-3}T\ln T + 0.159\times10^{-6}T^2 + 7.575T^{-1} + 63.728\times10^{-3}T$

952-1400 K: $\Delta Hf^\circ = -123.154 + 8.568\times10^{-3}T - 0.108\times10^{-6}T^2 + 44.750T^{-1}$

$\Delta Gf^\circ = -123.154 - 8.568\times10^{-3}T\ln T + 0.108\times10^{-6}T^2 + 22.375T^{-1} + 99.513\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Low-temperature heat capacities and entropy at 298 K from Taylor (237). High-temperature data based on Kaylor (115) and Marchidan (155).

CsCl(g)

Cesium Chloride (ideal gas)

[Formation: $Cs(c,l,g) + 0.5Cl_2(g) = CsCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.832	61.175	61.175	0	-57.400	-61.622	45.169
300	8.834	61.230	61.177	.016	-57.406	-61.648	44.910
301.55	8.835	61.276	61.177	.030	-57.410	-61.670	44.695
301.55	8.835	61.276	61.177	.030	-57.910	-61.670	44.695
400	8.922	63.785	61.522	.905	-58.194	-62.855	34.342
500	8.974	65.782	62.182	1.800	-58.474	-63.988	27.969
600	9.011	67.421	62.923	2.699	-58.751	-65.064	23.699
700	9.041	68.812	63.666	3.602	-59.028	-66.094	20.635
800	9.067	70.021	64.387	4.507	-59.306	-67.086	18.327
900	9.090	71.091	65.074	5.415	-59.582	-68.042	16.523
952	9.101	71.601	65.416	5.888	-59.726	-68.538	15.734
952	9.101	71.601	65.416	5.888	-75.924	-68.538	15.734
1000	9.112	72.049	65.724	6.325	-75.939	-68.166	14.897
1100	9.134	72.919	66.340	7.237	-75.973	-67.387	13.388
1200	9.154	73.715	66.922	8.152	-76.004	-66.604	12.130
1300	9.174	74.448	67.473	9.068	-76.036	-65.819	11.065
1400	9.194	75.129	67.996	9.986	-76.068	-65.033	10.152
1500	9.214	75.764	68.493	10.907	-76.097	-64.243	9.360
1600	9.233	76.359	68.966	11.829	-76.128	-63.452	8.667
1700	9.252	76.919	69.417	12.753	-76.159	-62.658	8.055
1800	9.271	77.449	69.849	13.680	-76.189	-61.864	7.511
1900	9.290	77.950	70.262	14.608	-76.221	-61.066	7.024
2000	9.309	78.427	70.658	15.538	-76.257	-60.267	6.586

Phase changes: 301.55 K, melting point of Cs; ΔH° = 0.500 kcal/mol.
952 K, boiling point of Cs to ideal monatomic gas; ΔH° = 16.198 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.938 + 0.188\times10^{-3}T - 0.144\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.938\times10^{-3}T + 0.094\times10^{-6}T^2 + 0.144\times10^{2}T^{-1} - 2.722$

Formation equations (kcal/mol):

298.15-301.55 K: $\Delta Hf^\circ = -57.072 + 1.388\times10^{-3}T - 7.597\times10^{-6}T^2 - 19.750T^{-1}$

$\Delta Gf^\circ = -57.072 - 1.388\times10^{-3}T\ln T + 7.597\times10^{-6}T^2 - 9.875T^{-1} - 9.502\times10^{-3}T$

301.55-952 K: $\Delta Hf^\circ = -57.216 - 2.609\times10^{-3}T - 0.065\times10^{-6}T^2 + 29.550T^{-1}$

$\Delta Gf^\circ = -57.216 + 2.609\times10^{-3}T\ln T + 0.065\times10^{-6}T^2 + 14.775T^{-1} - 29.845\times10^{-3}T$

952-2000 K: $\Delta Hf^\circ = -75.751 - 0.235\times10^{-3}T - 0.014\times10^{-6}T^2 + 59.150T^{-1}$

$\Delta Gf^\circ = -75.751 + 0.235\times10^{-3}T\ln T + 0.014\times10^{-6}T^2 + 29.575T^{-1} + 5.939\times10^{-3}T$

Source: Data from JANAF (60).

$(CsCl)_2(g)$

Dimeric Cesium Chloride (ideal gas)

[Formation: $2Cs(c,l,g) + Cl_2(g) = (CsCl)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.507	91.614	91.614	0	-157.700	-156.980	115.068
300	19.511	91.734	91.614	.036	-157.707	-156.974	114.354
301.55	19.513	91.835	91.615	.066	-157.713	-156.971	113.764
301.55	19.513	91.835	91.615	.066	-158.713	-156.971	113.764
400	19.667	97.372	92.382	1.996	-159.101	-156.345	85.422
500	19.740	101.769	93.835	3.967	-159.481	-155.612	68.017
600	19.780	105.372	95.467	5.943	-159.858	-154.802	56.386
700	19.804	108.423	97.106	7.922	-160.237	-153.929	48.058
800	19.820	111.069	98.689	9.904	-160.621	-153.004	41.798
900	19.831	113.404	100.197	11.886	-161.007	-152.028	36.917
952	19.835	114.518	100.949	12.918	-161.210	-151.528	34.786
952	19.835	114.518	100.949	12.918	-193.606	-151.528	34.786
1000	19.839	115.494	101.624	13.870	-193.559	-149.407	32.652
1100	19.844	117.385	102.972	15.854	-193.466	-144.996	28.808
1200	19.849	119.112	104.247	17.838	-193.374	-140.593	25.605
1300	19.852	120.700	105.452	19.823	-193.285	-136.197	22.896
1400	19.855	122.172	106.594	21.809	-193.199	-131.809	20.576
1500	19.857	123.542	107.679	23.794	-193.114	-127.427	18.566
1600	19.859	124.823	108.711	25.780	-193.034	-123.050	16.808
1700	19.860	126.027	109.694	27.766	-192.957	-118.677	15.257
1800	19.861	127.162	110.633	29.752	-192.886	-114.311	13.879
1900	19.862	128.236	111.532	31.738	-192.820	-109.948	12.647
2000	19.863	129.255	112.393	33.725	-192.764	-105.586	11.538

Phase changes: 301.55 K, melting point of Cs; $\Delta H°$ = 0.500 kcal/mol.

952 K, boiling point of Cs to ideal monatomic gas; $\Delta H°$ = 16.198 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.866 + 0.004\times10^{-3}T - 0.321\times10^{5}T^{-2}$

$H°- H°_{298} = 19.866\times10^{-3}T + 0.002\times10^{-6}T^{2} + 0.321\times10^{2}T^{-1} - 6.031$

Formation equations (kcal/mol):

298.15-301.55 K: $\Delta Hf° = -157.633 + 4.767\times10^{-3}T - 15.380\times10^{-6}T^{2} - 36.200T^{-1}$

$\Delta Gf° = -157.633 - 4.767\times10^{-3}T\ln T + 15.380\times10^{-6}T^{2} - 18.100T^{-1} + 24.969\times10^{-3}T$

301.55-952 K: $\Delta Hf° = -157.919 - 3.227\times10^{-3}T - 0.316\times10^{-6}T^{2} + 62.400T^{-1}$

$\Delta Gf° = -157.919 + 3.227\times10^{-3}T\ln T + 0.316\times10^{-6}T^{2} + 31.200T^{-1} - 15.719\times10^{-3}T$

952-2000 K: $\Delta Hf° = -194.990 + 1.521\times10^{-3}T - 0.214\times10^{-6}T^{2} + 121.600T^{-1}$

$\Delta Gf° = -194.990 - 1.521\times10^{-3}T\ln T + 0.214\times10^{-6}T^{2} + 60.800T^{-1} + 55.850\times10^{-3}T$

Source: Data from JANAF (60).

CsF(c,l)

Cesium Fluoride

[Formation: $Cs(c,l,g) + 0.5F_2(g) = CsF(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.210	22.230	22.230	0	-132.300	-125.633	92.090
300	12.218	22.306	22.230	.023	-132.298	-125.591	91.492
301.55	12.234	22.369	22.230	.042	-132.297	-125.556	90.996
301.55	12.234	22.369	22.230	.042	-132.797	-125.556	90.996
400	13.259	25.930	22.718	1.285	-132.682	-123.207	67.316
500	14.992	29.068	23.678	2.695	-132.423	-120.865	52.829
600	16.976	31.974	24.821	4.292	-131.984	-118.591	43.196
700	19.078	34.748	26.042	6.094	-131.346	-116.406	36.343
800	21.243	37.436	27.300	8.109	-130.501	-114.329	31.233
900	23.445	40.065	28.573	10.343	-129.442	-112.368	27.286
952	24.601	41.414	29.236	11.593	-128.805	-111.410	25.576
952	24.601	41.414	29.236	11.593	-145.003	-111.410	25.576
976	25.135	42.033	29.543	12.190	-144.631	-110.568	24.759
976	17.900	47.689	29.543	17.710	-139.111	-110.568	24.759
1000	17.900	48.124	29.984	18.140	-138.906	-109.869	24.011
1100	17.900	49.830	31.712	19.930	-138.056	-107.005	21.260
1200	17.900	51.388	33.288	21.720	-137.208	-104.220	18.981
1300	17.900	52.820	34.735	23.510	-136.362	-101.504	17.064
1400	17.900	54.147	36.076	25.300	-135.520	-98.855	15.432

Phase changes: 301.55 K, melting point of Cs; ΔH° = 0.500 kcal/mol.
952 K, boiling point of Cs to ideal monatomic gas; ΔH° = 16.198 kcal/mol.
976 K, melting point of CsF; ΔH° = 5.520 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-976 K: $Cp^\circ = 2.461 + 22.976\times10^{-3}T + 2.577\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 2.461\times10^{-3}T + 11.488\times10^{-6}T^2 - 2.577\times10^{2}T^{-1} - 0.891$

976-1400 K: $Cp^\circ = 17.900$

$H^\circ - H^\circ_{298} = 17.900\times10^{-3}T + 0.240$

Formation equations (kcal/mol):

298.15-301.55 K: $\Delta Hf^\circ = -130.131 - 4.929\times10^{-3}T + 3.754\times10^{-6}T^2 - 307.950T^{-1}$

$\Delta Gf^\circ = -130.131 + 4.929\times10^{-3}T\ln T - 3.754\times10^{-6}T^2 - 153.975T^{-1} - 10.145\times10^{-3}T$

301.55-952 K: $\Delta Hf^\circ = -130.274 - 8.926\times10^{-3}T + 11.286\times10^{-6}T^2 - 258.650T^{-1}$

$\Delta Gf^\circ = -130.274 + 8.926\times10^{-3}T\ln T - 11.286\times10^{-6}T^2 - 129.325T^{-1} - 30.488\times10^{-3}T$

952-976 K: $\Delta Hf^\circ = -148.810 - 6.552\times10^{-3}T + 11.337\times10^{-6}T^2 - 229.050T^{-1}$

$\Delta Gf^\circ = -148.810 + 6.552\times10^{-3}T\ln T - 11.337\times10^{-6}T^2 - 114.525T^{-1} + 5.296\times10^{-3}T$

976-1400 K: $\Delta Hf^\circ = -147.679 + 8.887\times10^{-3}T - 0.151\times10^{-6}T^2 + 28.650T^{-1}$

$\Delta Gf^\circ = -147.679 - 8.887\times10^{-3}T\ln T + 0.151\times10^{-6}T^2 + 14.325T^{-1} + 99.064\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Low-temperature heat capacities and entropy at 298 K from Paukov (191). High-temperature data based on Shpil'rain (214) and Macleod (149).

CsF(g)
Cesium Fluoride (ideal gas)
[Formation: $Cs(c,l,g) + 0.5F_2(g) = CsF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	8.565	58.102	58.102	0	-85.800	-89.828	65.845
300	8.570	58.155	58.102	.016	-85.805	-89.853	65.457
301.55	8.573	58.199	58.102	.029	-85.810	-89.874	65.136
301.55	8.573	58.199	58.102	.029	-86.310	-89.874	65.136
400	8.750	60.648	58.440	.883	-86.585	-90.997	49.718
500	8.848	62.612	59.086	1.763	-86.855	-92.069	40.243
600	8.909	64.231	59.813	2.651	-87.125	-93.086	33.906
700	8.952	65.608	60.545	3.544	-87.396	-94.058	29.366
800	8.985	66.806	61.255	4.441	-87.670	-94.993	25.950
900	9.012	67.865	61.931	5.341	-87.944	-95.890	23.285
952	9.024	68.372	62.268	5.811	-88.088	-96.357	22.120
952	9.024	68.372	62.268	5.811	-104.286	-96.357	22.120
1000	9.035	68.816	62.572	6.244	-104.302	-95.957	20.971
1100	9.056	69.678	63.180	7.148	-104.338	-95.120	18.898
1200	9.075	70.467	63.755	8.055	-104.373	-94.280	17.170
1300	9.093	71.194	64.299	8.963	-104.409	-93.437	15.708
1400	9.110	71.869	64.817	9.873	-104.447	-92.593	14.454
1500	9.126	72.498	65.308	10.785	-104.484	-91.745	13.367
1600	9.142	73.087	65.775	11.699	-104.522	-90.893	12.415
1700	9.158	73.642	66.222	12.614	-104.561	-90.040	11.575
1800	9.173	74.166	66.649	13.530	-104.603	-89.186	10.828
1900	9.187	74.662	67.058	14.448	-104.645	-88.328	10.160
2000	9.202	75.134	67.450	15.368	-104.692	-87.468	9.558

Phase changes: 301.55 K, melting point of Cs; $\Delta H° = 0.500$ kcal/mol.
952 K, boiling point of Cs to ideal monatomic gas; $\Delta H° = 16.198$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.912 + 0.154\times10^{-3}T - 0.349\times10^{5}T^{-2}$

$H°-H°_{298} = 8.912\times10^{-3}T + 0.077\times10^{-6}T^{2} + 0.349\times10^{2}T^{-1} - 2.781$

Formation equations (kcal/mol):

298.15-301.55 K: $\Delta Hf° = -85.522 + 1.522\times10^{-3}T - 7.657\times10^{-6}T^{2} - 15.350T^{-1}$

$\Delta Gf° = -85.522 - 1.522\times10^{-3}T\ln T + 7.657\times10^{-6}T^{2} - 7.675T^{-1} - 7.969\times10^{-3}T$

301.55-952 K: $\Delta Hf° = -85.665 - 2.475\times10^{-3}T - 0.125\times10^{-6}T^{2} + 33.950T^{-1}$

$\Delta Gf° = -85.665 + 2.475\times10^{-3}T\ln T + 0.125\times10^{-6}T^{2} + 16.975T^{-1} - 28.313\times10^{-3}T$

952-2000 K: $\Delta Hf° = -104.200 - 0.101\times10^{-3}T - 0.074\times10^{-6}T^{2} + 63.550T^{-1}$

$\Delta Gf° = -104.200 + 0.101\times10^{-3}T\ln T + 0.074\times10^{-6}T^{2} + 31.775T^{-1} + 7.471\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data from JANAF (60).

$(CsF)_2(g)$

Dimeric Cesium Fluoride (ideal gas)

[Formation: $2Cs(c,l,g) + F_2(g) = (CsF)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.093	84.179	84.179	0	-212.740	-211.248	154.847
300	19.103	84.297	84.180	.035	-212.747	-211.239	153.885
301.55	19.108	84.395	84.181	.065	-212.753	-211.231	153.089
301.55	19.108	84.395	84.181	.065	-213.753	-211.231	153.089
400	19.430	89.844	84.934	1.964	-214.111	-210.354	114.931
500	19.586	94.198	86.366	3.916	-214.461	-209.374	91.516
600	19.672	97.777	87.979	5.879	-214.812	-208.324	75.881
700	19.725	100.814	89.601	7.849	-215.170	-207.214	64.694
800	19.759	103.450	91.171	9.823	-215.538	-206.055	56.291
900	19.782	105.779	92.667	11.801	-215.909	-204.844	49.742
952	19.791	106.890	93.414	12.830	-216.107	-204.225	46.883
952	19.791	106.890	93.414	12.830	-248.503	-204.225	46.883
1000	19.799	107.864	94.084	13.780	-248.452	-201.993	44.145
1100	19.812	109.752	95.425	15.760	-248.352	-197.352	39.210
1200	19.821	111.476	96.691	17.742	-248.253	-192.718	35.098
1300	19.829	113.063	97.890	19.725	-248.159	-188.092	31.621
1400	19.835	114.533	99.027	21.708	-248.072	-183.477	28.642
1500	19.839	115.901	100.107	23.691	-247.986	-178.866	26.060
1600	19.843	117.182	101.134	25.676	-247.905	-174.260	23.803
1700	19.847	118.385	102.114	27.660	-247.829	-169.660	21.811
1800	19.849	119.519	103.050	29.645	-247.760	-165.063	20.041
1900	19.852	120.593	103.946	31.630	-247.696	-160.473	18.458
2000	19.854	121.611	104.803	33.615	-247.644	-155.882	17.034

Phase changes: 301.55 K, melting point of Cs; $\Delta H°$ = 0.500 kcal/mol.
952 K, boiling point of Cs to ideal monatomic gas; $\Delta H°$ = 16.198 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.856 + 0.010\times10^{-3}T - 0.681\times10^{5}T^{-2}$

$H°- H°_{298} = 19.856\times10^{-3}T + 0.005\times10^{-6}T^2 + 0.681\times10^{2}T^{-1} - 6.149$

Formation equations (kcal/mol):

298.15-301.55 K: $\Delta Hf° = -212.770 + 5.076\times10^{-3}T - 15.463\times10^{-6}T^2 - 32.400T^{-1}$

$\Delta Gf° = -212.770 - 5.076\times10^{-3}T\ln T + 15.463\times10^{-6}T^2 - 16.200T^{-1} + 29.598\times10^{-3}T$

301.55-952 K: $\Delta Hf° = -213.056 - 2.918\times10^{-3}T - 0.399\times10^{-6}T^2 + 66.200T^{-1}$

$\Delta Gf° = -213.056 + 2.918\times10^{-3}T\ln T + 0.399\times10^{-6}T^2 + 33.100T^{-1} - 11.090\times10^{-3}T$

952-2000 K: $\Delta Hf° = -250.127 + 1.830\times10^{-3}T - 0.297\times10^{-6}T^2 + 125.400T^{-1}$

$\Delta Gf° = -250.127 - 1.830\times10^{-3}T\ln T + 0.297\times10^{-6}T^2 + 62.700T^{-1} + 60.479\times10^{-3}T$

Source: Data from JANAF (60).

CsI(c,l)

Cesium Iodide

[Formation: $Cs(c,l,g) + 0.5I_2(c,l,g) = CsI(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.570	29.410	29.410	0	-82.840	-81.397	59.665
300	12.575	29.488	29.411	.023	-82.843	-81.388	59.290
301.55	12.579	29.553	29.412	.042	-82.846	-81.381	58.980
301.55	12.579	29.553	29.412	.042	-83.346	-81.381	58.980
386.8	12.782	32.712	29.803	1.125	-83.507	-80.805	45.656
386.8	12.782	32.712	29.803	1.125	-85.362	-80.805	45.656
400	12.814	33.141	29.906	1.294	-85.420	-80.649	44.064
458.4	12.989	34.896	30.433	2.046	-85.669	-79.934	38.109
458.4	12.989	34.896	30.433	2.046	-90.679	-79.934	38.109
500	13.113	36.030	30.852	2.589	-90.633	-78.960	34.513
600	13.583	38.459	31.922	3.922	-90.491	-76.638	27.915
700	14.258	40.601	33.012	5.312	-90.290	-74.344	23.211
800	15.150	42.561	34.085	6.781	-90.011	-72.085	19.692
900	16.265	44.408	35.130	8.350	-89.633	-69.865	16.965
900	16.750	51.208	35.130	14.470	-83.513	-69.865	16.965
952	16.750	52.148	36.034	15.341	-83.263	-69.095	15.862
952	16.750	52.148	36.034	15.341	-99.461	-69.095	15.862
1000	16.750	52.972	36.827	16.145	-99.112	-67.573	14.768
1100	16.750	54.569	38.369	17.820	-98.387	-64.454	12.806
1200	16.750	56.026	39.780	19.495	-97.663	-61.400	11.182
1300	16.750	57.367	41.082	21.170	-96.939	-58.407	9.819
1400	16.750	58.608	42.290	22.845	-96.218	-55.470	8.659

Phase changes: 301.55 K, melting point of Cs; ΔH° = 0.500 kcal/mol.
386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
900 K, melting point of CsI; ΔH° = 6.120 kcal/mol.
952 K, boiling point of Cs to ideal monatomic gas; ΔH° = 16.198 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-900 K: $Cp^\circ = 8.991 + 7.390\times10^{-3}T + 1.223\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.991\times10^{-3}T + 3.695\times10^{-6}T^2 - 1.223\times10^{2}T^{-1} - 2.599$

900-1400 K: $Cp^\circ = 16.750$

$H^\circ - H^\circ_{298} = 16.750\times10^{-3}T - 0.605$

CsI(c,l) - Continued

Formation equations (kcal/mol):

298.15-301.55 K: $\Delta Hf^\circ = -81.838 - 0.583\times10^{-3}T - 4.698\times10^{-6}T^2 - 122.300T^{-1}$

$\Delta Gf^\circ = -81.838 + 0.583\times10^{-3}T\ln T + 4.698\times10^{-6}T^2 - 61.150T^{-1} - 2.558\times10^{-3}T$

301.55-386.8 K: $\Delta Hf^\circ = -81.981 - 4.580\times10^{-3}T + 2.834\times10^{-6}T^2 - 73.000T^{-1}$

$\Delta Gf^\circ = -81.981 + 4.580\times10^{-3}T\ln T - 2.834\times10^{-6}T^2 - 36.500T^{-1} - 22.902\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -82.709 - 7.782\times10^{-3}T + 3.580\times10^{-6}T^2 - 73.000T^{-1}$

$\Delta Gf^\circ = -82.709 + 7.782\times10^{-3}T\ln T - 3.580\times10^{-6}T^2 - 36.500T^{-1} - 39.810\times10^{-3}T$

458.4-900 K: $\Delta Hf^\circ = -90.065 - 2.613\times10^{-3}T + 3.546\times10^{-6}T^2 - 80.650T^{-1}$

$\Delta Gf^\circ = -90.065 + 2.613\times10^{-3}T\ln T - 3.546\times10^{-6}T^2 - 40.325T^{-1} + 7.922\times10^{-3}T$

900-952 K: $\Delta Hf^\circ = -88.072 + 5.146\times10^{-3}T - 0.149\times10^{-6}T^2 + 41.650T^{-1}$

$\Delta Gf^\circ = -88.072 - 5.146\times10^{-3}T\ln T + 0.149\times10^{-6}T^2 + 20.825T^{-1} + 55.085\times10^{-3}T$

952-1400 K: $\Delta Hf^\circ = -106.607 + 7.521\times10^{-3}T - 0.098\times10^{-6}T^2 + 71.250T^{-1}$

$\Delta Gf^\circ = -106.607 - 7.521\times10^{-3}T\ln T + 0.098\times10^{-6}T^2 + 35.625T^{-1} + 90.869\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (255). Low-temperature heat capacities from Sorai (221). High-temperature data based on Kaylor (115).

CuBr(c,1)

Copper Monobromide

[Formation: $Cu(c,1) + 0.5Br_2(l,g) = CuBr(c,1)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	13.084	22.969	22.969	0	-25.240	-24.302	17.814
300	13.100	23.050	22.970	.024	-25.243	-24.297	17.700
332.6	13.311	24.412	23.046	.454	-25.299	-24.191	15.896
332.6	13.311	24.412	23.046	.454	-28.831	-24.191	15.896
400	13.746	26.911	23.491	1.368	-28.615	-23.272	12.715
500	14.414	30.029	24.497	2.766	-28.269	-21.977	9.606
600	18.919	32.921	25.656	4.359	-27.747	-20.760	7.562
657	33.288	35.135	26.375	5.755	-26.968	-20.126	6.695
657	17.500	36.809	26.375	6.855	-25.868	-20.126	6.695
700	17.500	37.918	27.051	7.607	-25.584	-19.759	6.169
741	17.500	38.914	27.679	8.325	-25.315	-19.425	5.729
741	13.900	39.602	27.679	8.835	-24.805	-19.425	5.729
759	13.900	39.936	27.966	9.085	-24.752	-19.295	5.556
759	15.136	41.543	27.966	10.305	-23.532	-19.295	5.556
800	14.862	42.332	28.682	10.920	-23.370	-19.070	5.210
900	14.283	44.048	30.297	12.376	-23.026	-18.555	4.506
1000	13.831	45.528	31.747	13.781	-22.747	-18.073	3.950
1100	13.506	46.830	33.060	15.147	-22.524	-17.616	3.500
1200	13.308	47.996	34.258	16.486	-22.352	-17.178	3.129
1300	13.237	49.058	35.356	17.812	-22.224	-16.755	2.817
1357.6	13.269	49.632	35.949	18.575	-22.172	-16.515	2.659
1357.6	13.269	49.632	35.949	18.575	-25.292	-16.515	2.659
1400	13.293	50.040	36.370	19.138	-25.252	-16.242	2.535
1500	13.477	50.963	37.313	20.475	-25.149	-15.603	2.273

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
657 K, α - β transition point of CuBr; $\Delta H°$ = 1.100 kcal/mo.
741 K, β - γ transition point of CuBr; $\Delta H°$ = 0.510 kcal/mol.
759 K, melting point of CuBr; $\Delta H°$ = 1.220 kcal/mol.
1357.6 K, melting point of Cu; $\Delta H°$ = 3.120 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-657 K: $Cp° = -12.428 + 49.340\times10^{-3}T + 9.601\times10^{5}T^{-2}$

$H°- H°_{298} = -12.428\times10^{-3}T + 24.670\times10^{-6}T^{2} - 9.601\times10^{2}T^{-1} + 4.733$

657-741 K: $Cp° = 17.501$

$H°- H°_{298} = 17.501\times10^{-3}T - 4.643$

741-759 K: $Cp° = 13.900$

$H°- H°_{298} = 13.900\times10^{-3}T - 1.465$

759-1500 K: $Cp° = 10.983 + 0.834\times10^{-3}T + 20.276\times10^{5}T^{-2}$

$H°- H°_{298} = 10.983\times10^{-3}T + 0.417\times10^{-6}T^{2} - 20.276\times10^{2}T^{-1} + 4.400$

CuBr(c,l) - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -16.180 - 26.794\times10^{-3}T + 23.910\times10^{-6}T^2 - 953.100T^{-1}$

$\Delta Gf^\circ = -16.180 + 26.794\times10^{-3}T\ln T - 23.910\times10^{-6}T^2 - 476.550T^{-1} - 167.411\times10^{-3}T$

332.6-657 K: $\Delta Hf^\circ = -21.180 - 22.213\times10^{-3}T + 23.833\times10^{-6}T^2 - 968.800T^{-1}$

$\Delta Gf^\circ = -21.180 + 22.213\times10^{-3}T\ln T - 23.833\times10^{-6}T^2 - 484.400T^{-1} - 125.733\times10^{-3}T$

657-741 K: $\Delta Hf^\circ = -30.556 + 7.716\times10^{-3}T - 0.838\times10^{-6}T^2 - 8.700T^{-1}$

$\Delta Gf^\circ = -30.556 - 7.716\times10^{-3}T\ln T + 0.838\times10^{-6}T^2 - 4.350T^{-1} + 65.387\times10^{-3}T$

741-759 K: $\Delta Hf^\circ = -27.378 + 4.115\times10^{-3}T - 0.838\times10^{-6}T^2 - 8.700T^{-1}$

$\Delta Gf^\circ = -27.378 - 4.115\times10^{-3}T\ln T + 0.838\times10^{-6}T^2 - 4.350T^{-1} + 37.302\times10^{-3}T$

759-1357.6 K: $\Delta Hf^\circ = -21.513 + 1.198\times10^{-3}T - 0.421\times10^{-6}T^2 - 2036.300T^{-1}$

$\Delta Gf^\circ = -21.513 - 1.198\times10^{-3}T\ln T + 0.421\times10^{-6}T^2 - 1018.150T^{-1} + 12.306\times10^{-3}T$

1357.6-1500 K: $\Delta Hf^\circ = -22.754 - 1.282\times10^{-3}T + 0.389\times10^{-6}T^2 - 2043.300T^{-1}$

$\Delta Gf^\circ = -22.754 + 1.282\times10^{-3}T\ln T - 0.389\times10^{-6}T^2 - 1021.650T^{-1} - 3.568\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Ko(134). Other data from Ferrante (78).

CuBr(g)

Copper Monobromide (ideal gas)

[Formation: $Cu(c,l) + 0.5Br_2(l,g) = CuBr(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.641	59.319	59.319	0	29.300	19.400	-14.220
300	8.645	59.372	59.319	.016	29.288	19.339	-14.088
332.6	8.694	60.266	59.368	.299	29.086	18.268	-12.004
332.6	8.694	60.266	59.368	.299	25.553	18.268	-12.004
400	8.794	61.882	59.660	.889	25.446	16.801	-9.179
500	8.875	63.854	60.308	1.773	25.278	14.658	-6.407
600	8.926	65.477	61.039	2.663	25.097	12.551	-4.572
700	8.962	66.856	61.775	3.557	24.906	10.474	-3.270
800	8.990	68.054	62.485	4.455	24.706	8.427	-2.302
900	9.013	69.114	63.164	5.355	24.493	6.405	-1.555
1000	9.033	70.065	63.808	6.257	24.269	4.406	-.963
1100	9.051	70.927	64.416	7.162	24.031	2.432	-.483
1200	9.068	71.715	64.992	8.068	23.771	.481	-.088
1300	9.084	72.441	65.537	8.975	23.479	-1.450	.244
1357.6	9.093	72.835	65.839	9.498	23.292	-2.553	.411
1357.6	9.093	72.835	65.839	9.498	20.172	-2.553	.411
1400	9.099	73.115	66.055	9.884	20.034	-3.261	.509
1500	9.113	73.743	66.546	10.795	19.711	-4.913	.716
1600	9.127	74.332	67.015	11.707	19.388	-6.544	.894
1700	9.141	74.886	67.462	12.620	19.066	-8.157	1.049
1800	9.155	75.409	67.890	13.535	18.746	-9.749	1.184
1900	9.168	75.904	68.298	14.451	18.426	-11.321	1.302
2000	9.182	76.375	68.690	15.369	18.107	-12.880	1.407

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
1357.6 K, melting point of Cu; ΔH° = 3.120 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.917 + 0.142\times10^{-3}T - 0.283\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.917\times10^{-3}T + 0.071\times10^{-6}T^2 + 0.283\times10^{2}T^{-1} - 2.760$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = 30.867 - 5.448\times10^{-3}T - 0.689\times10^{-6}T^2 + 35.300T^{-1}$

$\Delta Gf^\circ = 30.867 + 5.448\times10^{-3}T\ln T + 0.689\times10^{-6}T^2 + 17.650T^{-1} - 69.910\times10^{-3}T$

332.6-1357.6 K: $\Delta Hf^\circ = 25.867 - 0.868\times10^{-3}T - 0.766\times10^{-6}T^2 + 19.600T^{-1}$

$\Delta Gf^\circ = 25.867 + 0.868\times10^{-3}T\ln T + 0.766\times10^{-6}T^2 + 9.800T^{-1} - 28.232\times10^{-3}T$

1357.6-2000 K: $\Delta Hf^\circ = 24.626 - 3.348\times10^{-3}T + 0.044\times10^{-6}T^2 + 12.600T^{-1}$

$\Delta Gf^\circ = 24.626 + 3.348\times10^{-3}T\ln T - 0.044\times10^{-6}T^2 + 6.300T^{-1} - 44.106\times10^{-3}T$

Source: Data from King (128).

$(CuBr)_3(g)$

Trimeric Copper Monobromide (ideal gas)

[Formation: $3Cu(c) + 1.5Br_2(l,g) = (CuBr)_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	30.770	108.000	108.000	0	-36.200	-45.043	33.017
300	30.780	108.190	108.003	.056	-36.227	-45.098	32.853
332.6	30.878	111.370	108.180	1.061	-36.678	-46.039	30.251
332.6	30.878	111.370	108.180	1.061	-47.276	-46.039	30.251
400	31.080	117.088	109.213	3.150	-47.278	-45.792	25.019
500	31.320	124.051	111.509	6.271	-47.316	-45.420	19.853
600	31.490	129.776	114.091	9.411	-47.386	-45.032	16.403
700	31.600	134.639	116.688	12.566	-47.487	-44.632	13.935
800	31.680	138.864	119.201	15.730	-47.619	-44.215	12.079
900	31.720	142.598	121.598	18.900	-47.786	-43.781	10.631
1000	31.730	145.940	123.867	22.073	-47.991	-43.325	9.469
1100	31.740	148.965	126.013	25.247	-48.246	-42.844	8.512
1200	31.750	151.728	128.044	28.421	-48.572	-42.340	7.711
1300	31.760	154.269	129.964	31.597	-48.991	-41.807	7.028

Phase change: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $Cp^\circ = 31.760 + 0.080\times10^{-3}T - 1.090\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 31.760\times10^{-3}T + 0.040\times10^{-6}T^2 + 1.090\times10^{2}T^{-1} - 9.838$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -33.057 - 11.337\times10^{-3}T - 2.240\times10^{-6}T^2 + 130.000T^{-1}$

$\Delta Gf^\circ = -33.057 + 11.337\times10^{-3}T\ln T + 2.240\times10^{-6}T^2 + 65.000T^{-1} - 106.191\times10^{-3}T$

332.6-1300 K: $\Delta Hf^\circ = -48.058 + 2.405\times10^{-3}T - 2.473\times10^{-6}T^2 + 82.900T^{-1}$

$\Delta Gf^\circ = -48.058 - 2.405\times10^{-3}T\ln T + 2.473\times10^{-6}T^2 + 41.450T^{-1} + 18.841\times10^{-3}T$

Source: Data from King (128).

$CuBr_2(c)$
Copper Dibromide
[Formation: $Cu(c) + Br_2(l,g) = CuBr_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	18.100	30.800	30.800	0	-33.100	-29.074	21.312
300	18.100	30.912	30.800	.034	-33.110	-29.048	21.161
332.6	18.230	32.790	30.904	.627	-33.296	-28.598	18.791
332.6	18.230	32.790	30.904	.627	-40.361	-28.598	18.791
350	18.300	33.721	31.021	.945	-40.298	-27.984	17.474
400	18.400	36.173	31.516	1.863	-40.117	-26.240	14.337
450	18.600	38.353	32.157	2.788	-39.937	-24.518	11.907
500	18.700	40.316	32.876	3.720	-39.754	-22.814	9.972
550	18.800	42.102	33.635	4.657	-39.571	-21.128	8.395
600	18.900	43.742	34.410	5.599	-39.389	-19.459	7.088

Phase change: 332.6 K, boiling point of Br_2; $\Delta H^\circ = 7.065$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp^\circ = 18.250 + 1.240\times10^{-3}T - 0.460\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 18.250\times10^{-3}T + 0.620\times10^{-6}T^2 + 0.460\times10^{2}T^{-1} - 5.651$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -31.731 - 5.161\times10^{-3}T - 0.090\times10^{-6}T^2 + 53.000T^{-1}$

$\Delta Gf^\circ = -31.731 + 5.161\times10^{-3}T\ln T + 0.090\times10^{-6}T^2 + 26.500T^{-1} - 20.819\times10^{-3}T$

332.6-600 K: $\Delta Hf^\circ = -41.731 + 4.000\times10^{-3}T - 0.245\times10^{-6}T^2 + 21.600T^{-1}$

$\Delta Gf^\circ = -41.731 - 4.000\times10^{-3}T\ln T + 0.245\times10^{-6}T^2 + 10.800T^{-1} + 62.536\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Ko (134). Other data from King (128).

CuCl(c,l)

Copper Monochloride

[Formation: $Cu(c,l) + 0.5Cl_2(g) = CuCl(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.556	20.971	20.971	0	-37.200	-33.146	24.296
300	12.570	21.049	20.972	.023	-37.196	-33.121	24.128
400	13.151	24.748	21.470	1.311	-36.917	-31.803	17.376
500	13.859	27.755	22.437	2.659	-36.607	-30.561	13.358
600	15.602	30.388	23.545	4.106	-36.221	-29.385	10.703
685	27.078	32.978	24.543	5.778	-35.464	-28.457	9.079
685	19.000	34.679	24.543	6.943	-34.299	-28.457	9.079
696	19.000	34.982	24.706	7.152	-34.209	-28.364	8.906
696	14.829	37.414	24.706	8.845	-32.516	-28.364	8.906
700	14.793	37.500	24.779	8.905	-32.500	-28.340	8.848
800	14.100	39.426	26.492	10.347	-32.152	-27.771	7.587
900	13.690	41.061	28.023	11.734	-31.873	-27.241	6.615
1000	13.454	42.490	29.400	13.090	-31.640	-26.740	5.844
1100	13.334	43.766	30.649	14.429	-31.441	-26.258	5.217
1200	13.291	44.924	31.791	15.760	-31.275	-25.795	4.698
1300	13.303	45.988	32.843	17.089	-31.143	-25.345	4.261
1357.6	13.334	46.566	33.413	17.856	-31.086	-25.092	4.039
1357.6	13.334	46.566	33.413	17.856	-34.206	-25.092	4.039
1400	13.356	46.976	33.817	18.422	-34.163	-24.808	3.873
1500	13.438	47.900	34.726	19.761	-34.057	-24.144	3.518
1600	13.542	48.770	35.576	21.110	-33.942	-23.485	3.208
1700	13.664	49.595	36.377	22.470	-33.817	-22.837	2.936

Phase changes: 685 K, α - β transition point of CuCl; ΔH° = 1.165 kcal/mol.
696 K, melting point of CuCl; ΔH° = 1.693 kcal/mol.
1357.6 K, melting point of Cu; ΔH° = 3.120 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-685 K: $Cp^\circ = -1.830 + 29.034\times10^{-3}T + 5.093\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = -1.830\times10^{-3}T + 14.517\times10^{-6}T^2 - 5.093\times10^{2}T^{-1} + 0.963$

685-696 K: $Cp^\circ = 19.000$

$H^\circ - H^\circ_{298} = 19.000\times10^{-3}T - 6.072$

696-1700 K: $Cp^\circ = 9.560 + 2.028\times10^{-3}T + 18.685\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 9.560\times10^{-3}T + 1.014\times10^{-6}T^2 - 18.685\times10^{2}T^{-1} + 4.385$

Formation equations (kcal/mol):

298.15-685 K: $\Delta Hf^\circ = -33.168 - 11.564\times10^{-3}T + 13.663\times10^{-6}T^2 - 536.450T^{-1}$

$\Delta Gf^\circ = -33.168 + 11.564\times10^{-3}T\ln T - 13.663\times10^{-6}T^2 - 268.225T^{-1} - 58.720\times10^{-3}T$

685-696 K: $\Delta Hf^\circ = -40.203 + 9.266\times10^{-3}T - 0.854\times10^{-6}T^2 - 27.150T^{-1}$

$\Delta Gf^\circ = -40.203 - 9.266\times10^{-3}T\ln T + 0.854\times10^{-6}T^2 - 13.575T^{-1} + 77.072\times10^{-3}T$

696-1357.6 K: $\Delta Hf^\circ = -29.746 - 0.173\times10^{-3}T + 0.160\times10^{-6}T^2 - 1895.650T^{-1}$

$\Delta Gf^\circ = -29.746 + 0.173\times10^{-3}T\ln T - 0.160\times10^{-6}T^2 - 947.825T^{-1} + 2.894\times10^{-3}T$

1357.6-1700 K: $\Delta Hf^\circ = -30.987 - 2.654\times10^{-3}T + 0.970\times10^{-6}T^2 - 1902.650T^{-1}$

$\Delta Gf^\circ = -30.987 + 2.654\times10^{-3}T\ln T - 0.970\times10^{-6}T^2 - 951.325T^{-1} - 12.980\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from King (128). Low-temperature heat capacities and entropy at 298 K from Stuve (230). High-temperature data from Ferrante (78).

CuCl(g)
Copper Monochloride (ideal gas)
[Formation: $Cu(c,l) + 0.5Cl_2(g) = CuCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.427	56.664	56.664	0	21.800	15.212	-11.151
300	8.433	56.716	56.664	.016	21.798	15.172	-11.053
400	8.656	59.176	56.998	.871	21.643	12.986	-7.095
500	8.778	61.122	57.634	1.744	21.478	10.840	-4.738
600	8.853	62.729	58.354	2.625	21.299	8.729	-3.180
700	8.905	64.098	59.079	3.513	21.108	6.649	-2.076
800	8.942	65.290	59.783	4.406	20.907	4.597	-1.256
900	8.972	66.345	60.454	5.302	20.695	2.572	-.624
1000	8.996	67.291	61.091	6.200	20.471	.569	-.124
1100	9.017	68.150	61.695	7.101	20.231	-1.409	.280
1200	9.036	68.935	62.266	8.003	19.968	-3.365	.613
1300	9.053	69.659	62.807	8.908	19.676	-5.298	.891
1357.6	9.062	70.052	63.106	9.430	19.487	-6.404	1.031
1357.6	9.062	70.052	63.106	9.430	16.367	-6.404	1.031
1400	9.069	70.331	63.321	9.814	16.229	-7.113	1.110
1500	9.084	70.957	63.809	10.722	15.904	-8.769	1.278
1600	9.099	71.544	64.275	11.631	15.579	-10.403	1.421
1700	9.112	72.096	64.719	12.541	15.254	-12.018	1.545
1800	9.126	72.617	65.143	13.453	14.931	-13.612	1.653
1900	9.139	73.111	65.549	14.367	14.609	-15.188	1.747
2000	9.152	73.580	65.939	15.281	14.286	-16.749	1.830

Phase change: 1357.6 K, melting point of Cu; ΔH° = 3.120 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.930 + 0.120\times10^{-3}T - 0.520\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.930\times10^{-3}T + 0.060\times10^{-6}T^2 + 0.520\times10^{2}T^{-1} - 2.842$

Formation equations (kcal/mol):

298.15-1357.6 K: $\Delta Hf^\circ = 22.027 - 0.803\times10^{-3}T - 0.794\times10^{-6}T^2 + 24.850T^{-1}$

$\Delta Gf^\circ = 22.027 + 0.803\times10^{-3}T\ln T + 0.794\times10^{-6}T^2 + 12.425T^{-1} - 27.810\times10^{-3}T$

1357.6-2000 K: $\Delta Hf^\circ = 20.786 - 3.283\times10^{-3}T + 0.016\times10^{-6}T^2 + 17.850T^{-1}$

$\Delta Gf^\circ = 20.786 + 3.283\times10^{-3}T\ln T - 0.016\times10^{-6}T^2 + 8.925T^{-1} - 43.684\times10^{-3}T$

Source: Data from King (128).

$(CuCl)_3(g)$

Trimeric Copper Monochloride (ideal gas)

[Formation: $3Cu(c,l) + 1.5Cl_2(g) = (CuCl)_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	29.773	102.631	102.631	0	-58.900	-58.579	42.939
300	29.795	102.815	102.632	.055	-58.901	-58.577	42.673
400	30.621	111.515	103.813	3.081	-58.902	-58.470	31.946
500	31.028	118.397	106.065	6.166	-58.932	-58.361	25.509
600	31.256	124.076	108.608	9.281	-58.999	-58.239	21.213
700	31.396	128.905	111.171	12.414	-59.100	-58.105	18.141
800	31.488	133.104	113.655	15.559	-59.237	-57.955	15.832
900	31.552	136.817	116.027	18.711	-59.409	-57.784	14.032
1000	31.598	140.144	118.275	21.869	-59.620	-57.594	12.587
1100	31.632	143.157	120.402	25.030	-59.880	-57.377	11.400
1200	31.657	145.910	122.414	28.195	-60.210	-57.134	10.405
1300	31.678	148.445	124.321	31.361	-60.635	-56.866	9.560
1357.6	31.687	149.818	125.374	33.186	-60.940	-56.700	9.128
1357.6	31.687	149.818	125.374	33.186	-70.300	-56.700	9.128
1400	31.694	150.793	126.129	34.530	-70.525	-56.272	8.784
1500	31.707	152.980	127.847	37.700	-71.054	-55.236	8.048
1600	31.717	155.027	129.483	40.871	-71.585	-54.162	7.398
1700	31.726	156.950	131.042	44.043	-72.117	-53.059	6.821
1800	31.733	158.764	132.533	47.216	-72.650	-51.924	6.304
1900	31.740	160.480	133.959	50.390	-73.184	-50.754	5.838
2000	31.745	162.108	135.326	53.564	-73.723	-49.560	5.416

Phase change: 1357.6 K, melting point of Cu; $\Delta H^\circ = 3.120$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 31.694 + 0.062\times10^{-3}T - 1.725\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 31.694\times10^{-3}T + 0.031\times10^{-6}T^2 + 1.725\times10^{2}T^{-1} - 10.031$

Formation equations (kcal/mol):

298.15-1357.6 K: $\Delta Hf^\circ = -59.724 + 2.493\times10^{-3}T - 2.531\times10^{-6}T^2 + 91.050T^{-1}$

$\Delta Gf^\circ = -59.724 - 2.493\times10^{-3}T\ln T + 2.531\times10^{-6}T^2 + 45.525T^{-1} + 16.779\times10^{-3}T$

1357.6-2000 K: $\Delta Hf^\circ = -63.446 - 4.947\times10^{-3}T - 0.101\times10^{-6}T^2 + 70.050T^{-1}$

$\Delta Gf^\circ = -63.446 + 4.947\times10^{-3}T\ln T + 0.101\times10^{-6}T^2 + 35.025T^{-1} - 30.842\times10^{-3}T$

Source: Data from King (128).

$CuCl_2(c)$
Copper Dichloride
[Formation: $Cu(c) + Cl_2(g) = CuCl_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	17.178	25.830	25.830	0	-52.100	-41.550	30.457
300	17.206	25.936	25.830	.032	-52.094	-41.484	30.221
400	18.246	31.047	26.520	1.811	-51.739	-38.000	20.762
500	18.798	35.183	27.853	3.665	-51.350	-34.611	15.128
600	19.158	38.644	29.371	5.564	-50.946	-31.300	11.401
675	19.366	40.913	30.529	7.009	-50.637	-28.863	9.345
675	19.700	41.163	30.529	7.178	-50.468	-28.863	9.345
700	19.700	41.880	30.923	7.670	-50.357	-28.065	8.762
800	19.700	44.510	32.460	9.640	-49.924	-24.911	6.805
900	19.700	46.831	33.931	11.610	-49.507	-21.809	5.296

Phase change: 675 K, α - β transition point of $CuCl_2$; ΔH° = 0.169 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-675 K: $Cp^\circ = 18.851 + 1.370\times10^{-3}T - 1.852\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 18.851\times10^{-3}T + 0.685\times10^{-6}T^2 + 1.852\times10^{2}T^{-1} - 6.302$

675-900 K: $Cp^\circ = 19.700$

$H^\circ - H^\circ_{298} = 19.700\times10^{-3}T - 6.120$

Formation equations (kcal/mol):

298.15-675 K: $\Delta Hf^\circ = -53.899 + 4.704\times10^{-3}T - 0.213\times10^{-6}T^2 + 123.900T^{-1}$

$\Delta Gf^\circ = -53.899 - 4.704\times10^{-3}T\ln T + 0.213\times10^{-6}T^2 + 61.950T^{-1} + 67.459\times10^{-3}T$

675-900 K: $\Delta Hf^\circ = -53.717 + 5.553\times10^{-3}T - 0.898\times10^{-6}T^2 - 61.300T^{-1}$

$\Delta Gf^\circ = -53.717 - 5.553\times10^{-3}T\ln T + 0.898\times10^{-6}T^2 - 30.650T^{-1} + 72.461\times10^{-3}T$

Sources: Enthalpy of formation, entropy at 298 K, and low-temperature heat capacities from King (128). High-temperature data from Ferrante (78).

CuF(c)

Copper Monofluoride

[Formation: $Cu(c) + 0.5F_2(g) = CuF(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.400	15.500	15.500	0	-50.000	-45.037	33.013
300	12.420	15.577	15.500	.023	-49.995	-45.006	32.787
400	13.180	19.255	15.995	1.304	-49.693	-43.387	23.705
500	13.780	22.264	16.958	2.653	-49.358	-41.850	18.292
600	14.240	24.820	18.062	4.055	-48.996	-40.383	14.709
700	14.570	27.041	19.188	5.497	-48.618	-38.976	12.169
800	14.820	29.004	20.295	6.967	-48.229	-37.625	10.279
900	15.010	30.761	21.362	8.459	-47.836	-36.323	8.820
1000	15.140	32.349	22.382	9.967	-47.444	-35.064	7.663
1100	15.240	33.797	23.355	11.486	-47.060	-33.845	6.724
1200	15.310	35.126	24.282	13.013	-46.694	-32.660	5.948
1300	15.360	36.354	25.164	14.547	-46.353	-31.506	5.297

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $Cp^\circ = 14.370 + 0.980\times10^{-3}T - 2.430\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.370\times10^{-3}T + 0.490\times10^{-6}T^2 + 2.430\times10^{2}T^{-1} - 5.143$

Formation equations (kcal/mol):

298.15-1300 K: $\Delta Hf^\circ = -52.064 + 4.796\times10^{-3}T - 0.407\times10^{-6}T^2 + 199.750T^{-1}$

$\Delta Gf^\circ = -52.064 - 4.796\times10^{-3}T\ln T + 0.407\times10^{-6}T^2 + 99.875T^{-1} + 49.648\times10^{-3}T$

Source: Data from King (128).

CuF(g)
Copper Monofluoride (ideal gas)
[Formation: $Cu(c,l) + 0.5F_2(g) = CuF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	7.982	54.108	54.108	0	14.000	7.452	-5.462
300	7.990	54.158	54.108	.015	13.997	7.411	-5.399
400	8.341	56.508	54.425	.833	13.837	5.241	-2.863
500	8.555	58.394	55.038	1.678	13.668	3.110	-1.359
600	8.692	59.967	55.732	2.541	13.490	1.015	-.370
700	8.787	61.315	56.436	3.415	13.301	-1.049	.328
800	8.855	62.493	57.120	4.298	13.102	-3.086	.843
900	8.907	63.539	57.777	5.186	12.891	-5.096	1.237
1000	8.949	64.479	58.400	6.079	12.668	-7.082	1.548
1100	8.984	65.334	58.993	6.975	12.429	-9.046	1.797
1200	9.014	66.117	59.554	7.875	12.168	-10.987	2.001
1300	9.040	66.840	60.088	8.778	11.878	-12.906	2.170
1357.6	9.054	67.231	60.382	9.299	11.690	-14.003	2.254
1357.6	9.054	67.231	60.382	9.299	8.570	-14.003	2.254
1400	9.064	67.510	60.594	9.683	8.432	-14.706	2.296
1500	9.086	68.136	61.075	10.591	8.108	-16.347	2.382
1600	9.106	68.723	61.535	11.500	7.785	-17.966	2.454
1700	9.125	69.276	61.975	12.412	7.462	-19.567	2.515
1800	9.143	69.798	62.395	13.325	7.139	-21.147	2.568
1900	9.161	70.293	62.798	14.240	6.818	-22.710	2.612
2000	9.178	70.763	63.185	15.157	6.496	-24.256	2.650

Phase change: 1357.6 K, melting point of Cu; ΔH° = 3.120 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.860 + 0.180\times10^{-3}T - 0.940\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.860\times10^{-3}T + 0.090\times10^{-6}T^2 + 0.940\times10^{2}T^{-1} - 2.965$

Formation equations (kcal/mol):

298.15-1357.6 K: $\Delta Hf^\circ = 14.114 - 0.714\times10^{-3}T - 0.807\times10^{-6}T^2 + 50.750T^{-1}$

$\Delta Gf^\circ = 14.114 + 0.714\times10^{-3}T\ln T + 0.807\times10^{-6}T^2 + 25.375T^{-1} - 26.940\times10^{-3}T$

1357.6-2000 K: $\Delta Hf^\circ = 12.874 - 3.194\times10^{-3}T + 0.003\times10^{-6}T^2 + 43.750T^{-1}$

$\Delta Gf^\circ = 12.874 + 3.194\times10^{-3}T\ln T - 0.003\times10^{-6}T^2 + 21.875T^{-1} - 42.814\times10^{-3}T$

Source: Data from King (128).

CuF_2(c,l)

Copper Difluoride

[Formation: $Cu(c,l) + F_2(g) = CuF_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	15.813	18.650	18.650	0	-129.020	-117.775	86.330
300	15.848	18.748	18.651	.029	-129.016	-117.705	85.747
400	17.465	23.540	19.293	1.699	-128.709	-113.977	62.274
500	18.679	27.574	20.556	3.509	-128.315	-110.340	48.229
600	19.618	31.066	22.023	5.426	-127.854	-106.786	38.896
700	20.363	34.148	23.539	7.426	-127.341	-103.315	32.256
800	20.976	36.909	25.042	9.494	-126.786	-99.921	27.297
900	21.509	39.410	26.500	11.619	-126.195	-96.596	23.456
1000	22.015	41.703	27.908	13.795	-125.575	-93.342	20.400
1100	22.540	43.825	29.260	16.022	-124.926	-90.148	17.911
1109	22.590	44.009	29.379	16.225	-124.866	-89.865	17.709
1109*	24.000	55.912	29.379	29.425	-111.666	-89.865	17.709
1200	24.000	57.805	31.464	31.609	-110.945	-88.105	16.046
1300	24.000	59.726	33.565	34.009	-110.186	-86.234	14.497
1357.6	24.000	60.766	34.697	35.391	-109.772	-85.184	13.713
1357.6	24.000	60.766	34.697	35.391	-112.892	-85.184	13.713
1400	24.000	61.504	35.498	36.409	-112.587	-84.324	13.163
1500	24.000	63.160	37.287	38.809	-111.870	-82.331	11.995
1600	24.000	64.709	38.953	41.209	-111.156	-80.383	10.980
1700	24.000	66.164	40.512	43.609	-110.444	-78.482	10.089
1800	24.000	67.536	41.975	46.009	-109.736	-76.623	9.303
1900	24.000	68.833	43.355	48.409	-109.029	-74.801	8.604
2000	24.000	70.064	44.660	50.809	-108.326	-73.018	7.979

*Data for liquid estimated.

Phase changes: 1109 K, melting point of CuF_2; ΔH° = 13.200 kcal/mol.
1357.6 K, melting point of Cu; ΔH° = 3.120 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1109 K: $Cp^\circ = 16.987 + 5.356\times10^{-3}T - 2.463\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 16.987\times10^{-3}T + 2.678\times10^{-6}T^2 + 2.463\times10^{2}T^{-1} - 6.129$

1109-2000 K: $Cp^\circ = 24.000$

$H^\circ - H^\circ_{298} = 24.000\times10^{-3}T + 2.809$

Formation equations (kcal/mol):

298.15-1109 K: $\Delta Hf^\circ = -130.625 + 3.159\times10^{-3}T + 1.694\times10^{-6}T^2 + 152.800T^{-1}$

$\Delta Gf^\circ = -130.625 - 3.159\times10^{-3}T\ln T - 1.694\times10^{-6}T^2 + 76.400T^{-1} + 60.744\times10^{-3}T$

1109-1357.6 K: $\Delta Hf^\circ = -121.687 + 10.172\times10^{-3}T - 0.984\times10^{-6}T^2 - 93.500T^{-1}$

$\Delta Gf^\circ = -121.687 - 10.172\times10^{-3}T\ln T + 0.984\times10^{-6}T^2 - 46.750T^{-1} + 98.984\times10^{-3}T$

1357.6-2000 K: $\Delta Hf^\circ = -122.928 + 7.692\times10^{-3}T - 0.174\times10^{-6}T^2 - 100.500T^{-1}$

$\Delta Gf^\circ = -122.928 - 7.692\times10^{-3}T\ln T + 0.174\times10^{-6}T^2 - 50.250T^{-1} + 83.111\times10^{-3}T$

Sources: Enthalpy of formation at 298 K, entropy at 298 K, and low-temperature heat capacities from Beyer (13). High-temperature data for crystal based on Ehlert (75). Heat capacity of liquid estimated. Temperature and enthalpy of fusion from Ehlert (77).

$CuF_2(g)$
Copper Difluoride (ideal gas)
[Formation: $Cu(c,l) + F_2(g) = CuF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	12.340	60.966	60.966	0	-67.200	-68.571	50.263
300	12.360	61.042	60.966	.023	-67.202	-68.580	49.960
400	13.199	64.723	61.463	1.304	-67.284	-69.026	37.713
500	13.709	67.727	62.423	2.652	-67.352	-69.453	30.357
600	14.029	70.257	63.524	4.040	-67.420	-69.867	25.449
700	14.240	72.437	64.646	5.454	-67.493	-70.269	21.939
800	14.384	74.348	65.741	6.886	-67.574	-70.660	19.303
900	14.488	76.049	66.795	8.329	-67.665	-71.041	17.251
1000	14.564	77.579	67.797	9.782	-67.768	-71.411	15.607
1100	14.624	78.970	68.750	11.242	-67.886	-71.768	14.259
1200	14.673	80.245	69.656	12.707	-68.027	-72.115	13.134
1300	14.717	81.421	70.516	14.176	-68.199	-72.450	12.180
1357.6	14.741	82.059	70.992	15.025	-68.319	-72.639	11.693
1357.6	14.741	82.059	70.992	15.025	-71.439	-72.639	11.693
1400	14.758	82.513	71.334	15.650	-71.526	-72.675	11.345
1500	14.801	83.533	72.114	17.128	-71.731	-72.751	10.600
1600	14.846	84.490	72.859	18.610	-71.935	-72.812	9.946
1700	14.895	85.391	73.569	20.097	-72.136	-72.860	9.367
1800	14.949	86.244	74.250	21.589	-72.336	-72.898	8.851
1900	15.008	87.054	74.903	23.087	-72.531	-72.922	8.388
2000	15.072	87.825	75.529	24.591	-72.724	-72.938	7.970

Phase change: 1357.6 K, melting point of Cu; $\Delta H° = 3.120$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 14.470 + 0.300\times10^{-3}T - 2.180\times10^{5}T^{-2}$

$H°- H°_{298} = 14.470\times10^{-3}T + 0.150\times10^{-6}T^2 + 2.180\times10^{2}T^{-1} - 5.059$

Formation equations (kcal/mol):

298.15-1357.6 K: $\Delta Hf° = -67.735 + 0.642\times10^{-3}T - 0.834\times10^{-6}T^2 + 124.500T^{-1}$

$\Delta Gf° = -67.735 - 0.642\times10^{-3}T\ln T + 0.834\times10^{-6}T^2 + 62.250T^{-1} - 0.096\times10^{-3}T$

1357.6-2000 K: $\Delta Hf° = -68.976 - 1.838\times10^{-3}T - 0.024\times10^{-6}T^2 + 117.500T^{-1}$

$\Delta Gf° = -68.976 + 1.838\times10^{-3}T\ln T + 0.024\times10^{-6}T^2 + 58.750T^{-1} - 15.970\times10^{-3}T$

Source: Data from King (128).

CuI(c,1)

Copper Monoiodide

[Formation: $Cu(c,1) + 0.5I_2(c,1,g) = CuI(c,1)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.920	23.087	23.087	0	-16.200	-16.583	12.155
300	12.940	23.167	23.087	.024	-16.199	-16.585	12.082
386.8	13.572	26.533	23.495	1.175	-16.166	-16.701	9.437
386.8	13.572	26.533	23.495	1.175	-18.021	-16.701	9.437
400	13.668	26.990	23.602	1.355	-18.048	-16.656	9.100
458.4	14.140	28.848	24.156	2.151	-18.171	-16.445	7.840
458.4	14.140	28.848	24.156	2.151	-23.181	-16.445	7.840
500	14.477	30.091	24.599	2.746	-23.028	-15.839	6.923
600	18.400	32.951	25.751	4.320	-22.529	-14.443	5.261
642	30.787	34.515	26.270	5.293	-22.011	-13.892	4.729
642	33.100	35.667	26.270	6.033	-21.271	-13.892	4.729
680	33.100	37.570	26.848	7.291	-20.427	-13.479	4.332
680	16.400	38.502	26.849	7.924	-19.794	-13.479	4.332
700	16.400	38.977	27.188	8.252	-19.685	-13.295	4.151
800	16.400	41.167	28.802	9.892	-19.147	-12.419	3.393
868	16.400	42.505	29.823	11.007	-18.788	-11.862	2.987
868	15.903	44.688	29.823	12.903	-16.892	-11.862	2.987
900	15.714	45.261	30.363	13.408	-16.746	-11.680	2.836
1000	15.165	46.887	31.935	14.952	-16.330	-11.139	2.434
1100	14.681	48.310	33.361	16.444	-15.984	-10.637	2.113
1200	14.263	49.569	34.661	17.890	-15.707	-10.164	1.851
1300	13.910	50.696	35.851	19.298	-15.500	-9.712	1.633
1357.6	13.744	51.295	36.494	20.094	-15.416	-9.460	1.523
1357.6	13.744	51.295	36.494	20.094	-18.536	-9.460	1.523
1400	13.621	51.716	36.949	20.674	-18.481	-9.177	1.433
1500	13.398	52.648	37.965	22.025	-18.366	-8.518	1.241
1600	13.241	53.507	38.910	23.356	-18.272	-7.862	1.074

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
642 K, α - β transition point of CuI; ΔH° = 0.740 kcal/mol.
680 K, β - γ transition point of CuI; ΔH° = 0.633 kcal/mol.
868 K, melting point of CuI; ΔH° = 1.896 kcal/mol.
1357.6 K, melting point of Cu; ΔH° = 3.120 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-642 K: $Cp^\circ = -7.954 + 41.172\times10^{-3}T + 7.643\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = -7.954\times10^{-3}T + 20.586\times10^{-6}T^2 - 7.643\times10^{2}T^{-1} + 3.105$

642-680 K: $Cp^\circ = 33.100$

$H^\circ - H^\circ_{298} = 33.100\times10^{-3}T - 15.217$

680-868 K: $Cp^\circ = 16.400$

$H^\circ - H^\circ_{298} = 16.400\times10^{-3}T - 3.228$

868-1600 K: $Cp^\circ = 14.645 - 1.372\times10^{-3}T + 18.453\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.645\times10^{-3}T - 0.686\times10^{-6}T^2 - 18.453\times10^{2}T^{-1} + 2.834$

CuI(c,l) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -9.474 - 19.712\times10^{-3}T + 19.030\times10^{-6}T^2 - 757.300T^{-1}$
$\Delta Gf^\circ = -9.474 + 19.712\times10^{-3}T\ln T - 19.030\times10^{-6}T^2 - 378.650T^{-1} - 126.222\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -10.202 - 22.915\times10^{-3}T + 19.776\times10^{-6}T^2 - 757.300T^{-1}$
$\Delta Gf^\circ = -10.202 + 22.915\times10^{-3}T\ln T - 19.776\times10^{-6}T^2 - 378.650T^{-1} - 143.130\times10^{-3}T$

458.4-642 K: $\Delta Hf^\circ = -17.559 - 17.745\times10^{-3}T + 19.742\times10^{-6}T^2 - 764.950T^{-1}$
$\Delta Gf^\circ = -17.559 + 17.745\times10^{-3}T\ln T - 19.742\times10^{-6}T^2 - 382.475T^{-1} - 95.399\times10^{-3}T$

642-680 K: $\Delta Hf^\circ = -35.881 + 23.309\times10^{-3}T - 0.844\times10^{-6}T^2 - 0.650T^{-1}$
$\Delta Gf^\circ = -35.881 - 23.309\times10^{-3}T\ln T + 0.844\times10^{-6}T^2 - 0.325T^{-1} + 184.395\times10^{-3}T$

680-868 K: $\Delta Hf^\circ = -23.892 + 6.609\times10^{-3}T - 0.844\times10^{-6}T^2 - 0.650T^{-1}$
$\Delta Gf^\circ = -23.892 - 6.609\times10^{-3}T\ln T + 0.844\times10^{-6}T^2 - 0.325T^{-1} + 57.845\times10^{-3}T$

868-1357.6 K: $\Delta Hf^\circ = -17.830 + 4.855\times10^{-3}T - 1.530\times10^{-6}T^2 - 1845.950T-1$
$\Delta Gf^\circ = -17.830 - 4.855\times10^{-3}T\ln T + 1.530\times10^{-6}T^2 - 922.975T^{-1} + 39.615\times10^{-3}T$

1357.6-1600 K: $\Delta Hf^\circ = -19.071 + 2.375\times10^{-3}T - 0.720\times10^{-6}T^2 - 1852.950T^{-1}$
$\Delta Gf^\circ = -19.071 - 2.375\times10^{-3}T\ln T + 0.720\times10^{-6}T^2 - 926.475T^{-1} + 23.742\times10^{-3}T$

Sources: Enthalpy of formation at 298 K, entropy at 298 K, and low-temperature heat capacities from King (128). High-temperature data from Ferrante (78).

CuI(g)

Copper Monoiodide (ideal gas)

[Formation: $Cu(c,l) + 0.5I_2(c,l,g) = CuI(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.727	61.088	61.088	0	34.000	22.287	-16.337
300	8.730	61.142	61.089	.016	33.993	22.215	-16.183
386.8	8.830	63.374	61.360	.779	33.638	18.852	-10.652
386.8	8.830	63.374	61.360	.779	31.783	18.852	-10.652
400	8.845	63.671	61.431	.896	31.693	18.413	-10.060
458.4	8.881	64.879	61.797	1.413	31.292	16.501	-7.867
458.4	8.881	64.879	61.797	1.413	26.281	16.501	-7.867
500	8.906	65.652	62.086	1.783	26.209	15.617	-6.826
600	8.945	67.280	62.820	2.676	26.027	13.516	-4.923
700	8.974	68.661	63.558	3.572	25.835	11.446	-3.574
800	8.996	69.861	64.272	4.471	25.633	9.405	-2.569
900	9.016	70.922	64.954	5.371	25.417	7.388	-1.794
1000	9.033	71.872	65.598	6.274	25.192	5.399	-1.180
1100	9.048	72.734	66.209	7.178	24.951	3.431	-.682
1200	9.063	73.522	66.786	8.083	24.686	1.485	-.270
1300	9.076	74.248	67.333	8.990	24.393	-.437	.074
1357.6	9.084	74.642	67.634	9.514	24.204	-1.535	.247
1357.6	9.084	74.642	67.634	9.514	21.084	-1.535	.247
1400	9.090	74.921	67.850	9.899	20.945	-2.239	.350
1500	9.103	75.548	68.343	10.808	20.617	-3.885	.566
1600	9.115	76.136	68.812	11.719	20.291	-5.506	.752
1700	9.128	76.689	69.259	12.631	19.965	-7.110	.914
1800	9.140	77.211	69.686	13.545	19.641	-8.692	1.055
1900	9.152	77.706	70.096	14.459	19.315	-10.258	1.180
2000	9.164	78.176	70.489	15.375	18.991	-11.807	1.290

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
1357.6 K, melting point of Cu; ΔH° = 3.120 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.940 + 0.120\times10^{-3}T - 0.240\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.940\times10^{-3}T + 0.060\times10^{-6}T^2 + 0.240\times10^{2}T^{-1} - 2.751$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = 34.869 - 2.819\times10^{-3}T - 1.496\times10^{-6}T^2 + 31.000T^{-1}$

$\Delta Gf^\circ = 34.869 + 2.819\times10^{-3}T\ln T + 1.496\times10^{-6}T^2 + 15.500T^{-1} - 58.880\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = 34.142 - 6.021\times10^{-3}T - 0.750\times10^{-6}T^2 + 31.000T^{-1}$

$\Delta Gf^\circ = 34.142 + 6.021\times10^{-3}T\ln T + 0.750\times10^{-6}T^2 + 15.500T^{-1} - 75.788\times10^{-3}T$

458.4-1357.6 K: $\Delta Hf^\circ = 26.785 - 0.851\times10^{-3}T - 0.784\times10^{-6}T^2 + 23.350T^{-1}$

$\Delta Gf^\circ = 26.785 + 0.851\times10^{-3}T\ln T + 0.784\times10^{-6}T^2 + 11.675T^{-1} - 28.056\times10^{-3}T$

1357.6-2000 K: $\Delta Hf^\circ = 25.544 - 3.331\times10^{-3}T + 0.026\times10^{-6}T^2 + 16.350T^{-1}$

$\Delta Gf^\circ = 25.544 + 3.331\times10^{-3}T\ln T - 0.026\times10^{-6}T^2 + 8.175T^{-1} - 43.930\times10^{-3}T$

Source: Data from King (128).

$(CuI)_3(g)$

Trimeric Copper Monoiodide (ideal gas)

[Formation: $3Cu(c) + 1.5I_2(c,l,g) = (CuI)_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	31.020	111.000	111.000	0	-4.000	-17.593	12.896
300	31.030	111.192	111.002	.057	-4.012	-17.677	12.878
386.8	31.230	119.104	111.969	2.760	-4.665	-21.551	12.176
386.8	31.230	119.104	111.969	2.760	-10.229	-21.551	12.176
400	31.260	120.152	112.222	3.172	-10.437	-21.934	11.984
458.4	31.365	124.420	113.511	5.001	-11.363	-23.548	11.227
458.4	31.365	124.420	113.511	5.001	-26.395	-23.548	11.227
500	31.440	127.148	114.534	6.307	-26.415	-23.286	10.178
600	31.560	132.891	117.128	9.458	-26.488	-22.653	8.251
700	31.650	137.764	119.737	12.619	-26.592	-22.005	6.870
800	31.700	141.993	122.260	15.786	-26.729	-21.340	5.830
900	31.720	145.728	124.664	18.958	-26.903	-20.656	5.016
1000	31.730	149.071	126.941	22.130	-27.116	-19.951	4.360
1100	31.730	152.095	129.092	25.303	-27.380	-19.221	3.819
1200	31.730	154.856	131.126	28.476	-27.715	-18.465	3.363
1300	31.740	157.396	133.051	31.649	-28.143	-17.681	2.972

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $Cp^\circ = 31.830 - 0.020\times10^{-3}T - 0.860\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 31.830\times10^{-3}T - 0.010\times10^{-6}T^2 + 0.860\times10^{2}T^{-1} - 9.778$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -2.916 - 3.445\times10^{-3}T - 4.678\times10^{-6}T^2 + 107.000T^{-1}$

$\Delta Gf^\circ = -2.916 + 3.445\times10^{-3}T\ln T + 4.678\times10^{-6}T^2 + 53.500T^{-1} - 70.855\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -5.098 - 13.052\times10^{-3}T - 2.440\times10^{-6}T^2 + 107.000T^{-1}$

$\Delta Gf^\circ = -5.098 + 13.052\times10^{-3}T\ln T + 2.440\times10^{-6}T^2 + 53.500T^{-1} - 121.578\times10^{-3}T$

458.4-1300 K: $\Delta Hf^\circ = -27.168 + 2.459\times10^{-3}T - 2.542\times10^{-6}T^2 + 84.050T^{-1}$

$\Delta Gf^\circ = -27.168 - 2.459\times10^{-3}T\ln T + 2.542\times10^{-6}T^2 + 42.025T^{-1} + 21.616\times10^{-3}T$

Source: Data from King (128).

$DyBr_3(g)$

Dysprosium Tribromide (ideal gas)

[Formation: $Dy(c,l) + 1.5Br_2(l,g) = DyBr_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.093	96.555	96.555	0	-129.100	-136.281	99.896
300	19.102	96.673	96.556	.035	-129.126	-136.325	99.312
332.6	19.208	98.649	96.666	.659	-129.603	-137.084	90.076
332.6	19.208	98.649	96.666	.659	-140.201	-137.084	90.076
400	19.426	102.219	97.309	1.964	-140.233	-136.454	74.554
500	19.589	106.573	98.743	3.915	-140.277	-135.505	59.228
600	19.696	110.154	100.354	5.880	-140.319	-134.545	49.007
700	19.788	113.197	101.977	7.854	-140.367	-133.575	41.703
800	19.881	115.845	103.549	9.837	-140.426	-132.602	36.225
900	19.978	118.193	105.049	11.830	-140.499	-131.618	31.961
1000	20.077	120.303	106.470	13.833	-140.590	-130.630	28.549
1100	20.174	122.221	107.816	15.846	-140.708	-129.629	25.755
1200	20.265	123.980	109.090	17.868	-140.868	-128.613	23.423
1300	20.347	125.605	110.299	19.898	-141.081	-127.583	21.448
1400	20.418	127.116	111.447	21.937	-141.352	-126.540	19.754
1500	20.478	128.527	112.539	23.982	-141.695	-125.468	18.280
1600	20.527	129.850	113.580	26.032	-142.116	-124.379	16.989
1657	20.549	130.569	114.152	27.203	-142.391	-123.730	16.319
1657	20.549	130.569	114.152	27.203	-143.386	-123.730	16.319
1682	20.559	130.877	114.399	27.717	-143.381	-123.434	16.038
1682	20.559	130.877	114.399	27.717	-146.024	-123.434	16.038
1700	20.566	131.096	114.574	28.087	-146.114	-123.204	15.839
1800	20.595	132.272	115.525	30.145	-146.615	-121.826	14.792
1900	20.615	133.386	116.435	32.206	-147.115	-120.442	13.854
2000	20.628	134.444	117.310	34.268	-147.617	-119.032	13.007

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.
1657 K, α - β transition point of Dy; $\Delta H° = 0.995$ kcal/mol.
1682 K, melting point of Dy; $\Delta H° = 2.643$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.445 + 0.680\times10^{-3}T - 0.493\times10^{5}T^{-2}$

$H°- H°_{298} = 19.445\times10^{-3}T + 0.340\times10^{-6}T^2 + 0.493\times10^{2}T^{-1} - 5.993$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -126.345 - 11.181\times10^{-3}T - 1.735\times10^{-6}T^2 + 218.500T^{-1}$

$\Delta Gf° = -126.345 + 11.181\times10^{-3}T\ln T + 1.735\times10^{-6}T^2 + 109.250T^{-1} - 98.781\times10^{-3}T$

332.6-1657 K: $\Delta Hf° = -141.345 + 2.560\times10^{-3}T - 1.967\times10^{-6}T^2 + 171.400T^{-1}$

$\Delta Gf° = -141.345 - 2.560\times10^{-3}T\ln T + 1.967\times10^{-6}T^2 + 85.700T^{-1} + 26.251\times10^{-3}T$

1657-1682 K: $\Delta Hf° = -143.028 - 0.650\times10^{-3}T + 0.257\times10^{-6}T^2 + 2.200T^{-1}$

$\Delta Gf° = -143.028 + 0.650\times10^{-3}T\ln T - 0.257\times10^{-6}T^2 + 1.100T^{-1} + 7.190\times10^{-3}T$

1682-2000 K: $\Delta Hf° = -136.875 - 5.880\times10^{-3}T + 0.257\times10^{-6}T^2 + 2.200T^{-1}$

$\Delta Gf° = -136.875 + 5.880\times10^{-3}T\ln T - 0.257\times10^{-6}T^2 + 1.100T^{-1} - 35.316\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166) and Hurtgen (103). Other data based on Myers (165) and Dieke (56).

$DyCl_3(c,l)$
Dysprosium Trichloride
[Formation: $Dy(c) + 1.5Cl_2(g) = DyCl_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	23.200	36.800	36.800	0	-236.600	-218.402	160.091
300	23.223	36.944	36.801	.043	-236.592	-218.290	159.022
400	24.131	43.762	37.725	2.415	-236.137	-212.258	115.971
500	24.697	49.211	39.495	4.858	-235.645	-206.344	90.192
600	25.146	53.755	41.503	7.351	-235.131	-200.532	73.043
700	25.554	57.662	43.539	9.886	-234.596	-194.803	60.819
800	25.952	61.100	45.524	12.461	-234.049	-189.159	51.675
900	26.356	64.180	47.428	15.077	-233.486	-183.576	44.578
924	26.455	64.876	47.874	15.710	-233.350	-182.248	43.106
924	34.600	71.483	47.874	21.815	-227.245	-182.248	43.106
1000	34.600	74.218	49.773	24.445	-226.203	-178.594	39.031
1100	34.600	77.516	52.148	27.905	-224.866	-173.899	34.550
1200	34.600	80.526	54.389	31.365	-223.583	-169.321	30.837
1300	34.600	83.296	56.508	34.825	-222.362	-164.849	27.713

*Entropy and heat capacity at 298 K estimated.

Phase change: 924 K, melting point of $DyCl_3$; ΔH° = 6.105 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-924 K: $Cp^\circ = 23.588 + 3.184\times10^{-3}T - 1.189\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 23.588\times10^{-3}T + 1.592\times10^{-6}T^2 + 1.189\times10^{2}T^{-1} - 7.573$

924-1300 K: $Cp^\circ = 34.600$

$H^\circ - H^\circ_{298} = 34.600\times10^{-3}T - 10.155$

Formation equations (kcal/mol):

298.15-924 K: $\Delta Hf^\circ = -239.199 + 6.857\times10^{-3}T - 0.765\times10^{-6}T^2 + 185.650T^{-1}$

$\Delta Gf^\circ = -239.199 - 6.857\times10^{-3}T\ln T + 0.765\times10^{-6}T^2 + 92.825T^{-1} + 107.552\times10^{-3}T$

924-1300 K: $\Delta Hf^\circ = -241.781 + 17.869\times10^{-3}T - 2.357\times10^{-6}T^2 + 66.750T^{-1}$

$\Delta Gf^\circ = -241.781 - 17.869\times10^{-3}T\ln T + 2.357\times10^{-6}T^2 + 33.375T^{-1} + 184.143\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Kim (122). Entropy and heat capacity at 298 K estimated. High-temperature data based on Dworkin (69).

$DyCl_3(g)$

Dysprosium Trichloride (ideal gas)

[Formation: $Dy(c,l) + 1.5Cl_2(g) = DyCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	18.677	89.956	89.956	0	-161.900	-159.551	116.952
300	18.690	90.071	89.956	.035	-161.899	-159.536	116.220
400	19.174	95.523	90.696	1.931	-161.921	-158.747	86.734
500	19.421	99.831	92.107	3.862	-161.941	-157.950	69.039
600	19.577	103.386	93.699	5.812	-161.969	-157.149	57.241
700	19.699	106.413	95.304	7.776	-162.005	-156.338	48.810
800	19.813	109.051	96.861	9.752	-162.057	-155.529	42.488
900	19.924	111.391	98.348	11.739	-162.123	-154.703	37.567
1000	20.033	113.496	99.760	13.736	-162.212	-153.881	33.630
1100	20.138	115.411	101.097	15.745	-162.326	-153.044	30.407
1200	20.234	117.167	102.364	17.764	-162.484	-152.192	27.718
1300	20.321	118.790	103.565	19.792	-162.695	-151.324	25.440
1400	20.396	120.299	104.708	21.827	-162.967	-150.447	23.486
1500	20.459	121.708	105.795	23.870	-163.309	-149.537	21.787
1600	20.510	123.030	106.831	25.919	-163.729	-148.611	20.299
1657	20.533	123.749	107.401	27.089	-164.005	-148.052	19.527
1657	20.533	123.749	107.401	27.089	-165.000	-148.052	19.527
1682	20.543	124.056	107.646	27.602	-164.995	-147.798	19.204
1682	20.543	124.056	107.646	27.602	-167.638	-147.798	19.204
1700	20.550	124.275	107.821	27.972	-167.727	-147.597	18.975
1800	20.581	125.450	108.768	30.028	-168.231	-146.385	17.773
1900	20.603	126.564	109.676	32.088	-168.732	-145.165	16.698
2000	20.617	127.621	110.547	34.149	-169.236	-143.916	15.726

Phase changes: 1657 K, α - β transition point of Dy; ΔH° = 0.995 kcal/mol.
1682 K, melting point of Dy; ΔH° = 2.643 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.420 + 0.692\times10^{-3}T - 0.844\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.420\times10^{-3}T + 0.346\times10^{-6}T^2 + 0.844\times10^{2}T^{-1} - 6.104$

Formation equations (kcal/mol):

298.15-1657 K: $\Delta Hf^\circ = -163.030 + 2.689\times10^{-3}T - 2.011\times10^{-6}T^2 + 151.150T^{-1}$

$\Delta Gf^\circ = -163.030 - 2.689\times10^{-3}T\ln T + 2.011\times10^{-6}T^2 + 75.575T^{-1} + 25.543\times10^{-3}T$

1657-1682 K: $\Delta Hf^\circ = -164.713 - 0.520\times10^{-3}T + 0.214\times10^{-6}T^2 - 18.050T^{-1}$

$\Delta Gf^\circ = -164.713 + 0.520\times10^{-3}T\ln T - 0.214\times10^{-6}T^2 - 9.025T^{-1} + 6.482\times10^{-3}T$

1682-2000 K: $\Delta Hf^\circ = -158.559 - 5.750\times10^{-3}T + 0.214\times10^{-6}T^2 - 18.050T^{-1}$

$\Delta Gf^\circ = -158.559 + 5.750\times10^{-3}T\ln T - 0.214\times10^{-6}T^2 - 9.025T^{-1} - 36.024\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (167). Other data based on Myers (165) and Dieke (56).

$DyF_3(c,l)$
Dysprosium Trifluoride
[Formation: $Dy(c,l) + 1.5F_2(g) = DyF_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	22.500	28.400	28.400	0	-404.400	-385.866	282.844
300	22.529	28.539	28.399	.042	-404.391	-385.751	281.016
400	23.674	35.195	29.300	2.358	-403.900	-379.610	207.407
500	24.409	40.560	31.032	4.764	-403.372	-373.598	163.297
600	25.014	45.065	33.005	7.236	-402.820	-367.695	133.931
700	25.578	48.964	35.014	9.765	-402.246	-361.882	112.983
800	26.134	52.416	36.977	12.351	-401.652	-356.159	97.297
900	26.696	55.526	38.868	14.992	-401.036	-350.503	85.113
1000	27.268	58.368	40.678	17.690	-400.402	-344.927	75.383
1100	27.850	60.994	42.407	20.446	-399.753	-339.411	67.434
1200	28.441	63.443	44.059	23.261	-399.102	-333.954	60.821
1300	29.038	65.743	45.639	26.135	-398.456	-328.548	55.233
1400	29.636	67.917	47.154	29.068	-397.824	-323.204	50.454
1430	29.815	68.547	47.596	29.960	-397.637	-321.606	49.151
1430	37.500	78.337	47.596	43.960	-383.637	-321.606	49.151
1500	37.500	80.129	49.072	46.585	-382.688	-318.589	46.418
1600	37.500	82.550	51.091	50.335	-381.404	-314.365	42.940
1657	37.500	83.862	52.195	52.472	-380.710	-311.972	41.147
1657	37.500	83.862	52.195	52.472	-381.705	-311.972	41.147
1682	37.500	84.424	52.670	53.410	-381.276	-310.925	40.399
1682	37.500	84.424	52.670	53.410	-383.919	-310.925	40.399
1700	37.500	84.823	53.008	54.085	-383.703	-310.157	39.873
1800	37.500	86.966	54.835	57.835	-382.514	-305.851	37.135
1900	37.500	88.994	56.581	61.585	-381.327	-301.633	34.695
2000	37.500	90.918	58.250	65.335	-380.146	-297.475	32.506

*Entropy and heat capacity at 298 K estimated.

Phase changes: 1430 K, melting point of DyF_3; ΔH° = 14.000 kcal/mol.
1657 K, α - β transition point of Dy; ΔH° = 0.995 kcal/mol.
1682 K, melting point of Dy; ΔH° = 2.643 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1430 K: $Cp^\circ = 22.207 + 5.240\times10^{-3}T - 1.126\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 22.207\times10^{-3}T + 2.620\times10^{-6}T^2 + 1.126\times10^{2}T^{-1} - 7.232$
1430-2000 K: $Cp^\circ = 37.500$
$H^\circ - H^\circ_{298} = 37.500\times10^{-3}T - 9.665$

Formation equations (kcal/mol):

298.15-1430 K: $\Delta Hf^\circ = -406.627 + 5.955\times10^{-3}T + 0.134\times10^{-6}T^2 + 131.050T^{-1}$
$\Delta Gf^\circ = -406.627 - 5.955\times10^{-3}T\ln T - 0.134\times10^{-6}T^2 + 65.525T^{-1} + 102.866\times10^{-3}T$
1430-1657 K: $\Delta Hf^\circ = -409.060 + 21.248\times10^{-3}T - 2.486\times10^{-6}T^2 + 18.450T^{-1}$
$\Delta Gf^\circ = -409.060 - 21.248\times10^{-3}T\ln T + 2.486\times10^{-6}T^2 + 9.225T^{-1} + 211.958\times10^{-3}T$
1657-1682 K: $\Delta Hf^\circ = -410.743 + 18.038\times10^{-3}T - 0.261\times10^{-6}T^2 - 150.750T^{-1}$
$\Delta Gf^\circ = -410.743 - 18.038\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 - 75.375T^{-1} + 192.896\times10^{-3}T$
1682-2000 K: $\Delta Hf^\circ = -404.589 + 12.808\times10^{-3}T - 0.261\times10^{-6}T^2 - 150.750T^{-1}$
$\Delta Gf^\circ = -404.589 - 12.808\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 - 75.375T^{-1} + 150.391\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Johnson (111). Entropy and heat capacity at 298 K estimated. High-temperature data based on Spedding (222).

$DyF_3(g)$

Dysprosium Trifluoride (ideal gas)

[Formation: $Dy(c,l) + 1.5F_2(g) = DyF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	17.044	81.501	81.501	0	-297.700	-294.998	216.236
300	17.069	81.606	81.501	.032	-297.701	-294.981	214.891
400	18.076	86.669	82.184	1.794	-297.764	-294.064	160.667
500	18.652	90.770	83.504	3.633	-297.804	-293.134	128.127
600	19.015	94.205	85.010	5.517	-297.840	-292.198	106.432
700	19.274	97.156	86.539	7.432	-297.880	-291.249	90.931
800	19.480	99.744	88.032	9.370	-297.934	-290.302	79.306
900	19.658	102.048	89.462	11.327	-298.001	-289.338	70.260
1000	19.815	104.128	90.827	13.301	-298.091	-288.376	63.024
1100	19.956	106.023	92.123	15.290	-298.209	-287.399	57.100
1200	20.081	107.765	93.355	17.292	-298.371	-286.410	52.162
1300	20.189	109.377	94.527	19.305	-298.586	-285.403	47.980
1400	20.282	110.877	95.642	21.329	-298.863	-284.387	44.394
1500	20.359	112.279	96.705	23.361	-299.212	-283.338	41.282
1600	20.423	113.595	97.720	25.400	-299.639	-282.272	38.556
1657	20.451	114.310	98.278	26.565	-299.918	-281.632	37.145
1657	20.451	114.310	98.278	26.565	-300.913	-281.632	37.145
1682	20.464	114.616	98.518	27.077	-300.909	-281.342	36.556
1682	20.464	114.616	98.518	27.077	-303.552	-281.342	36.556
1700	20.473	114.834	98.690	27.445	-303.643	-281.116	36.139
1800	20.512	116.006	99.620	29.495	-304.155	-279.763	33.967
1900	20.541	117.115	100.511	31.547	-304.665	-278.401	32.023
2000	20.561	118.170	101.369	33.602	-305.179	-277.013	30.270

Phase changes: 1657 K, α - β transition point of Dy; $\Delta H° = 0.995$ kcal/mol.
1682 K, melting point of Dy; $\Delta H° = 2.643$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.045 + 0.916\times10^{-3}T - 2.021\times10^{5}T^{-2}$

$H°- H°_{298} = 19.045\times10^{-3}T + 0.458\times10^{-6}T^2 + 2.021\times10^{2}T^{-1} - 6.397$

Formation equations (kcal/mol):

298.15-1657 K: $\Delta Hf° = -299.092 + 2.793\times10^{-3}T - 2.028\times10^{-6}T^2 + 220.550T^{-1}$

$\Delta Gf° = -299.092 - 2.793\times10^{-3}T\ln T + 2.028\times10^{-6}T^2 + 110.275T^{-1} + 27.801\times10^{-3}T$

1657-1682 K: $\Delta Hf° = -300.775 - 0.417\times10^{-3}T + 0.197\times10^{-6}T^2 + 51.350T^{-1}$

$\Delta Gf° = -300.775 + 0.417\times10^{-3}T\ln T - 0.197\times10^{-6}T^2 + 25.675T^{-1} + 8.739\times10^{-3}T$

1682-2000 K: $\Delta Hf° = -294.621 - 5.647\times10^{-3}T + 0.197\times10^{-6}T^2 + 51.350T^{-1}$

$\Delta Gf° = -294.621 + 5.647\times10^{-3}T\ln T - 0.197\times10^{-6}T^2 + 25.675T^{-1} - 33.766\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

$DyI_3(g)$

Dysprosium Triiodide (ideal gas)

[Formation: $Dy(c,l) + 1.5I_2(c,l,g) = DyI_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	19.473	103.341	103.341	0	-79.400	-92.460	67.774
300	19.478	103.462	103.342	.036	-79.412	-92.541	67.415
386.8	19.625	108.433	103.951	1.734	-80.110	-96.255	54.385
386.8	19.625	108.433	103.951	1.734	-85.673	-96.255	54.385
400	19.647	109.092	104.110	1.993	-85.885	-96.613	52.786
458.4	19.698	111.773	104.917	3.143	-86.815	-98.110	46.775
458.4	19.698	111.773	104.917	3.143	-101.846	-98.110	46.775
500	19.734	113.486	105.560	3.963	-101.864	-97.767	42.733
600	19.798	117.090	107.190	5.940	-101.908	-96.945	35.312
700	19.863	120.146	108.829	7.922	-101.957	-96.110	30.006
800	19.939	122.804	110.414	9.912	-102.018	-95.272	26.027
900	20.024	125.157	111.923	11.911	-102.092	-94.420	22.928
1000	20.115	127.271	113.353	13.918	-102.187	-93.566	20.448
1100	20.205	129.193	114.708	15.934	-102.310	-92.700	18.418
1200	20.291	130.955	115.990	17.958	-102.476	-91.820	16.722
1300	20.369	132.582	117.204	19.992	-102.692	-90.920	15.285
1400	20.437	134.094	118.357	22.032	-102.971	-90.011	14.051
1500	20.495	135.506	119.453	24.079	-103.319	-89.071	12.978
1600	20.542	136.830	120.498	26.131	-103.745	-88.111	12.035
1657	20.563	137.550	121.073	27.302	-104.026	-87.536	11.545
1657	20.563	137.550	121.073	27.302	-105.021	-87.536	11.545
1682	20.572	137.858	121.320	27.817	-105.017	-87.274	11.340
1682	20.572	137.858	121.320	27.817	-107.660	-87.274	11.340
1700	20.579	138.077	121.496	28.187	-107.751	-87.068	11.193
1800	20.606	139.254	122.451	30.246	-108.261	-85.823	10.420
1900	20.626	140.368	123.364	32.308	-108.770	-84.570	9.728
2000	20.638	141.427	124.242	34.371	-109.280	-83.288	9.101

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
1657 K, α - β transition point of Dy; ΔH° = 0.995 kcal/mol.
1682 K, melting point of Dy; ΔH° = 2.643 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.518 + 0.620\times10^{-3}T - 0.204\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.518\times10^{-3}T + 0.310\times10^{-6}T^2 + 0.204\times10^{2}T^{-1} - 5.915$

$DyI_3(g)$ - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -78.687 - 3.288\times10^{-3}T - 4.153\times10^{-6}T^2 + 189.600T^{-1}$

$\Delta Gf^\circ = -78.687 + 3.288\times10^{-3}T\ln T + 4.153\times10^{-6}T^2 + 94.800T^{-1} - 67.232\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -80.869 - 12.894\times10^{-3}T - 1.915\times10^{-6}T^2 + 189.600T^{-1}$

$\Delta Gf^\circ = -80.869 + 12.894\times10^{-3}T\ln T + 1.915\times10^{-6}T^2 + 94.800T^{-1} - 117.955\times10^{-3}T$

458.4-1657 K: $\Delta Hf^\circ = -102.939 + 2.616\times10^{-3}T - 2.017\times10^{-6}T^2 + 166.650T^{-1}$

$\Delta Gf^\circ = -102.939 - 2.616\times10^{-3}T\ln T + 2.017\times10^{-6}T^2 + 83.325T^{-1} + 25.239\times10^{-3}T$

1657-1682 K: $\Delta Hf^\circ = -104.622 - 0.594\times10^{-3}T + 0.208\times10^{-6}T^2 - 2.550T^{-1}$

$\Delta Gf^\circ = -104.622 + 0.594\times10^{-3}T\ln T - 0.208\times10^{-6}T^2 - 1.275T^{-1} + 6.177\times10^{-3}T$

1682-2000 K: $\Delta Hf^\circ = -98.468 - 5.824\times10^{-3}T + 0.208\times10^{-6}T^2 - 2.550T^{-1}$

$\Delta Gf^\circ = -98.468 + 5.824\times10^{-3}T\ln T - 0.208\times10^{-6}T^2 - 1.275T^{-1} - 36.328\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166) and Schumm (207). Other data based on Myers (165) and Dieke (56).

$ErBr_3(g)$
Erbium Tribromide (ideal gas)
[Formation: $Er(c,l) + 1.5Br_2(l,g) = ErBr_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	19.083	96.409	96.409	0	-130.500	-137.760	100.980
300	19.092	96.527	96.410	.035	-130.526	-137.805	100.389
332.6	19.199	98.502	96.520	.659	-131.004	-138.571	91.053
332.6	19.199	98.502	96.520	.659	-141.601	-138.571	91.053
400	19.419	102.071	97.163	1.963	-141.637	-137.956	75.375
500	19.578	106.423	98.595	3.914	-141.693	-137.031	59.895
600	19.666	110.001	100.208	5.876	-141.755	-136.094	49.571
700	19.720	113.037	101.828	7.846	-141.828	-135.141	42.192
800	19.755	115.672	103.397	9.820	-141.915	-134.185	36.657
900	19.779	118.000	104.893	11.796	-142.023	-133.211	32.348
1000	19.797	120.085	106.310	13.775	-142.150	-132.222	28.897
1100	19.810	121.973	107.649	15.756	-142.301	-131.224	26.071
1200	19.820	123.697	108.916	17.737	-142.479	-130.208	23.714
1300	19.827	125.284	110.115	19.720	-142.685	-129.173	21.716
1400	19.834	126.753	111.251	21.703	-142.925	-128.123	20.001
1500	19.838	128.122	112.331	23.686	-143.200	-127.071	18.514
1600	19.843	129.402	113.358	25.670	-143.513	-125.971	17.207
1700	19.846	130.605	114.337	27.655	-143.864	-124.863	16.052
1795	19.849	131.685	115.228	29.540	-144.238	-123.792	15.072
1795	19.849	131.685	115.228	29.540	-148.995	-123.792	15.072
1800	19.849	131.740	115.274	29.639	-149.010	-123.732	15.023
1900	19.851	132.813	116.169	31.624	-149.319	-122.317	14.069
2000	19.853	133.831	117.026	33.610	-149.629	-120.878	13.209

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
1795 K, melting point of Er; ΔH° = 4.757 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.841 + 0.020\times10^{-3}T - 0.679\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.841\times10^{-3}T + 0.010\times10^{-6}T^2 + 0.679\times10^{2}T^{-1} - 6.144$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -127.083 - 12.575\times10^{-3}T - 1.099\times10^{-6}T^2 + 128.200T^{-1}$

$\Delta Gf^\circ = -127.083 + 12.575\times10^{-3}T\ln T + 1.099\times10^{-6}T^2 + 64.100T^{-1} - 108.510\times10^{-3}T$

332.6-1795 K: $\Delta Hf^\circ = -142.084 + 1.166\times10^{-3}T - 1.332\times10^{-6}T^2 + 81.100T^{-1}$

$\Delta Gf^\circ = -142.084 - 1.166\times10^{-3}T\ln T + 1.332\times10^{-6}T^2 + 40.550T^{-1} + 16.522\times10^{-3}T$

1795-2000 K: $\Delta Hf^\circ = -143.737 - 2.804\times10^{-3}T - 0.072\times10^{-6}T^2 + 20.800T^{-1}$

$\Delta Gf^\circ = -143.737 + 2.804\times10^{-3}T\ln T + 0.072\times10^{-6}T^2 + 10.400T^{-1} - 10.033\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166) and Hurtgen (103). Other data based on Myers (165) and Dieke (56).

$ErCl_3(c,l)$

Erbium Trichloride

[Formation: $Er(c) + 1.5Cl_2(g) = ErCl_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	23.400	36.500	36.500	0	-237.700	-219.535	160.922
300	23.500	36.645	36.502	.043	-237.691	-219.423	159.847
400	24.200	43.496	37.428	2.427	-237.229	-213.400	116.595
500	24.700	48.954	39.208	4.873	-236.745	-207.500	90.697
600	25.300	53.512	41.222	7.374	-236.240	-201.699	73.468
700	25.800	57.444	43.264	9.926	-235.708	-195.980	61.187
800	26.200	60.914	45.258	12.525	-235.157	-190.350	52.001
900	26.700	64.030	47.173	15.171	-234.581	-184.780	44.870
1000	27.200	66.867	49.003	17.864	-233.986	-179.275	39.180
1049	27.400	68.171	49.868	19.200	-233.687	-176.602	36.793
1049	33.700	75.607	49.868	27.000	-225.887	-176.602	36.793
1100	33.700	77.207	51.099	28.719	-225.255	-174.223	34.615
1200	33.700	80.139	53.398	32.089	-224.039	-169.637	30.895
1300	33.700	82.837	55.561	35.459	-222.854	-165.147	27.763

*Data except enthalpy of formation at 298 K estimated 298-1049 K.

Phase change: 1049 K, melting point of $ErCl_3$; ΔH° = 7.800 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1049 K: $Cp^\circ = 22.731 + 4.482\times10^{-3}T - 0.560\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 22.731\times10^{-3}T + 2.241\times10^{-6}T^2 + 0.560\times10^{2}T^{-1} - 7.164$

1049-1300 K: $Cp^\circ = 33.700$

$H^\circ - H^\circ_{298} = 33.700\times10^{-3}T - 8.351$

Formation equations (kcal/mol):

298.15-1049 K: $\Delta Hf^\circ = -239.077 + 4.211\times10^{-3}T + 0.850\times10^{-6}T^2 + 13.850T^{-1}$

$\Delta Gf^\circ = -239.077 - 4.211\times10^{-3}T\ln T - 0.850\times10^{-6}T^2 + 6.925T^{-1} + 89.710\times10^{-3}T$

1049-1300 K: $\Delta Hf^\circ = -240.264 + 15.179\times10^{-3}T - 1.391\times10^{-6}T^2 - 42.150T^{-1}$

$\Delta Gf^\circ = -240.264 - 15.179\times10^{-3}T\ln T + 1.391\times10^{-6}T^2 - 21.075T^{-1} + 164.812\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Fuger (84). Entropy at 298 K estimated. High-temperature data from 298-1049 K estimated. Data at 1049 K, enthalpy of fusion, and heat capacity of liquid based on Dworkin (68).

$ErCl_3(g)$
Erbium Trichloride (ideal gas)
[Formation: $Er(c,l) + 1.5Cl_2(g) = ErCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	18.671	89.894	89.894	0	-161.100	-158.855	116.442
300	18.684	90.010	89.894	.035	-161.100	-158.841	115.714
400	19.170	95.460	90.635	1.930	-161.126	-158.083	86.371
500	19.412	99.767	92.045	3.861	-161.157	-157.319	68.763
600	19.548	103.319	93.637	5.809	-161.204	-156.548	57.022
700	19.632	106.339	95.240	7.769	-161.266	-155.763	48.631
800	19.687	108.964	96.795	9.735	-161.347	-154.980	42.338
900	19.726	111.286	98.279	11.706	-161.447	-154.175	37.438
1000	19.753	113.365	99.685	13.680	-161.570	-153.358	33.516
1100	19.774	115.249	101.016	15.656	-161.718	-152.532	30.305
1200	19.789	116.970	102.275	17.634	-161.894	-151.689	27.626
1300	19.801	118.555	103.467	19.614	-162.099	-150.825	25.356
1400	19.811	120.023	104.599	21.594	-162.339	-149.950	23.408
1500	19.819	121.390	105.673	23.576	-162.612	-149.068	21.719
1600	19.825	122.669	106.695	25.558	-162.925	-148.142	20.235
1700	19.831	123.871	107.670	27.541	-163.277	-147.202	18.924
1795	19.835	124.950	108.557	29.425	-163.652	-146.297	17.812
1795	19.835	124.950	108.557	29.425	-168.409	-146.297	17.812
1800	19.835	125.005	108.603	29.524	-168.424	-146.245	17.756
1900	19.839	126.077	109.494	31.508	-168.734	-145.002	16.679
2000	19.842	127.095	110.349	33.492	-169.048	-143.736	15.706

Phase change: 1795 K, melting point of Er; ΔH° = 4.757 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.806 + 0.040\times10^{-3}T - 1.020\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.806\times10^{-3}T + 0.020\times10^{-6}T^2 + 1.020\times10^{2}T^{-1} - 6.249$

Formation equations (kcal/mol):

298.15-1795 K: $\Delta Hf^\circ = -161.562 + 1.285\times10^{-3}T - 1.371\times10^{-6}T^2 + 59.850T^{-1}$

$\Delta Gf^\circ = -161.562 - 1.285\times10^{-3}T\ln T + 1.371\times10^{-6}T^2 + 29.925T^{-1} + 15.660\times10^{-3}T$

1795-2000 K: $\Delta Hf^\circ = -163.216 - 2.684\times10^{-3}T - 0.112\times10^{-6}T^2 - 0.450T^{-1}$

$\Delta Gf^\circ = -163.216 + 2.684\times10^{-3}T\ln T + 0.112\times10^{-6}T^2 - 0.225T^{-1} - 10.896\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166) and Fuger (84). Other data based on Myers (165) and Dieke (56).

$ErF_3(c,l)$

Erbium Trifluoride

[Formation: $Er(c,l) + 1.5F_2(g) = ErF_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	23.000	28.100	28.100	0	-404.800	-386.298	283.161
300	23.023	28.242	28.100	.043	-404.790	-386.184	281.331
400	23.917	35.003	29.015	2.395	-404.267	-380.057	207.651
500	24.469	40.402	30.772	4.815	-403.736	-374.068	163.503
600	24.917	44.904	32.762	7.285	-403.203	-368.185	134.110
700	25.340	48.777	34.780	9.798	-402.666	-362.388	113.141
800	25.771	52.188	36.747	12.353	-402.122	-356.678	97.439
900	26.226	55.250	38.636	14.953	-401.565	-351.027	85.240
1000	26.712	58.038	40.438	17.600	-400.994	-345.439	75.495
1100	27.236	60.608	42.156	20.297	-400.405	-339.914	67.534
1200	27.799	63.002	43.795	23.048	-399.794	-334.442	60.909
1300	28.403	65.250	45.359	25.858	-399.159	-329.014	55.312
1390	28.983	67.171	46.710	28.440	-398.568	-324.180	50.970
1390	32.240	72.250	46.710	35.500	-391.508	-324.180	50.970
1400	32.240	72.481	46.894	35.822	-391.409	-323.697	50.531
1419	32.240	72.915	47.238	36.435	-391.221	-322.778	49.713
1419	33.250	77.545	47.238	43.005	-384.651	-322.778	49.713
1500	33.250	79.391	48.926	45.698	-383.783	-319.283	46.519
1600	33.250	81.537	50.898	49.023	-382.750	-315.003	43.027
1700	33.250	83.553	52.760	52.348	-381.758	-310.796	39.955
1795	33.250	85.361	54.438	55.507	-380.860	-306.856	37.361
1795	33.250	85.361	54.438	55.507	-385.617	-306.856	37.361
1800	33.250	85.453	54.524	55.673	-385.565	-306.646	37.231
1900	33.250	87.251	56.199	58.998	-384.536	-302.291	34.771
2000	33.250	88.957	57.796	62.323	-383.512	-297.979	32.561

*Entropy and heat capacity at 298 K estimated.

Phase changes: 1390 K, α - β transition point of ErF_3; ΔH° = 7.060 kcal/mol.
1419 K, melting point of ErF_3; ΔH° = 6.750 kcal/mol.
1795 K, melting point of Er; ΔH° = 4.757 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1390 K: $Cp^\circ = 22.337 + 4.574\times10^{-3}T - 0.623\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 22.337\times10^{-3}T + 2.287\times10^{-6}T^2 + 0.623\times10^{2}T^{-1} - 7.072$

1390-1419 K: $Cp^\circ = 32.240$

$H^\circ - H^\circ_{298} = 32.240\times10^{-3}T - 9.314$

1419-2000 K: $Cp^\circ = 33.250$

$H^\circ - H^\circ_{298} = 33.250\times10^{-3}T - 4.177$

ErF_3(c,l) - Continued

Formation equations (kcal/mol):

298.15-1390 K: $\Delta Hf^\circ = -406.054 + 4.295\times10^{-3}T + 0.767\times10^{-6}T^2 - 28.150T^{-1}$

$\Delta Gf^\circ = -406.054 - 4.295\times10^{-3}T\ln T - 0.767\times10^{-6}T^2 - 14.075T^{-1} + 91.120\times10^{-3}T$

1390-1419 K: $\Delta Hf^\circ = -408.296 + 14.198\times10^{-3}T - 1.520\times10^{-6}T^2 - 90.450T^{-1}$

$\Delta Gf^\circ = -408.296 - 14.198\times10^{-3}T\ln T + 1.520\times10^{-6}T^2 - 45.225T^{-1} + 161.238\times10^{-3}T$

1419-1795 K: $\Delta Hf^\circ = -403.159 + 15.208\times10^{-3}T - 1.520\times10^{-6}T^2 - 90.450T^{-1}$

$\Delta Gf^\circ = -403.159 - 15.208\times10^{-3}T\ln T + 1.520\times10^{-6}T^2 - 45.225T^{-1} + 164.948\times10^{-3}T$

1795-2000 K: $\Delta Hf^\circ = -404.813 + 11.238\times10^{-3}T - 0.261\times10^{-6}T^2 - 150.750T^{-1}$

$\Delta Gf^\circ = -404.813 - 11.238\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 - 75.375T^{-1} + 138.393\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Johnson (111). Entropy and heat capacity at 298 K estimated. High-temperature data based on Spedding (222).

$ErF_3(g)$

Erbium Trifluoride (ideal gas)

[Formation: $Er(c,l) + 1.5F_2(g) = ErF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	16.972	81.262	81.262	0	-297.500	-294.849	216.127
300	16.997	81.367	81.264	.031	-297.502	-294.833	214.783
400	18.023	86.412	81.945	1.787	-297.576	-293.928	160.593
500	18.607	90.502	83.258	3.622	-297.629	-293.011	128.073
600	18.960	93.928	84.760	5.501	-297.688	-292.084	106.390
700	19.186	96.869	86.285	7.409	-297.755	-291.141	90.897
800	19.339	99.442	87.772	9.336	-297.840	-290.199	79.278
900	19.446	101.726	89.197	11.276	-297.942	-289.232	70.234
1000	19.525	103.779	90.555	13.224	-298.070	-288.257	62.998
1100	19.583	105.643	91.843	15.180	-298.222	-287.269	57.074
1200	19.628	107.349	93.065	17.141	-298.402	-286.265	52.135
1300	19.664	108.921	94.225	19.105	-298.612	-285.239	47.952
1400	19.692	110.380	95.328	21.073	-298.858	-284.204	44.366
1500	19.715	111.739	96.377	23.043	-299.138	-283.160	41.256
1600	19.734	113.012	97.377	25.016	-299.458	-282.070	38.529
1700	19.749	114.209	98.333	26.990	-299.816	-280.969	36.121
1795	19.761	115.283	99.201	28.867	-300.200	-279.906	34.079
1795	19.761	115.283	99.201	28.867	-304.957	-279.906	34.079
1800	19.762	115.338	99.246	28.966	-304.973	-279.846	33.978
1900	19.773	116.407	100.122	30.942	-305.292	-278.443	32.028
2000	19.783	117.421	100.961	32.920	-305.615	-277.011	30.270

Phase change: 1795 K, melting point of Er; $\Delta H° = 4.757$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.428 + 0.260\times10^{-3}T - 2.253\times10^{5}T^{-2}$

$H°-H°_{298} = 19.428\times10^{-3}T + 0.130\times10^{-6}T^2 + 2.253\times10^{2}T^{-1} - 6.560$

Formation equations (kcal/mol):

298.15-1795 K: $\Delta Hf° = -298.242 + 1.386\times10^{-3}T - 1.390\times10^{-6}T^2 + 134.850T^{-1}$

$\Delta Gf° = -298.242 - 1.386\times10^{-3}T\ln T + 1.390\times10^{-6}T^2 + 67.425T^{-1} + 18.105\times10^{-3}T$

1795-2000 K: $\Delta Hf° = -299.896 - 2.584\times10^{-3}T - 0.131\times10^{-6}T^2 + 74.550T^{-1}$

$\Delta Gf° = -299.896 + 2.584\times10^{-3}T\ln T + 0.131\times10^{-6}T^2 + 37.275T^{-1} - 8.451\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

$ErI_3(g)$
Erbium Triiodide (ideal gas)
[Formation: $Er(c,l) + 1.5I_2(c,l,g) = ErI_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	19.465	103.131	103.131	0	-81.200	-94.320	69.137
300	19.470	103.251	103.131	.036	-81.212	-94.401	68.770
386.8	19.619	108.220	103.738	1.734	-81.913	-98.127	55.443
386.8	19.619	108.220	103.738	1.734	-87.476	-98.127	55.443
400	19.642	108.879	103.896	1.993	-87.689	-98.487	53.810
458.4	19.690	111.560	104.705	3.142	-88.625	-99.997	47.675
458.4	19.690	111.560	104.705	3.142	-103.657	-99.997	47.675
500	19.724	113.272	105.348	3.962	-103.680	-99.661	43.561
600	19.769	116.873	106.980	5.936	-103.743	-98.855	36.007
700	19.796	119.922	108.615	7.915	-103.817	-98.030	30.606
800	19.814	122.567	110.198	9.895	-103.907	-97.204	26.554
900	19.826	124.901	111.704	11.877	-104.017	-96.357	23.398
1000	19.835	126.990	113.130	13.860	-104.147	-95.494	20.870
1100	19.841	128.881	114.477	15.844	-104.302	-94.625	18.800
1200	19.846	130.608	115.751	17.828	-104.486	-93.738	17.072
1300	19.850	132.196	116.955	19.813	-104.697	-92.826	15.605
1400	19.853	133.668	118.098	21.798	-104.943	-91.905	14.347
1500	19.855	135.037	119.181	23.784	-105.223	-90.977	13.255
1600	19.857	136.319	120.213	25.769	-105.542	-90.003	12.294
1700	19.859	137.523	121.197	27.755	-105.901	-89.019	11.444
1795	19.860	138.603	122.089	29.642	-106.282	-88.066	10.722
1795	19.860	138.603	122.089	29.642	-111.039	-88.066	10.722
1800	19.860	138.658	122.135	29.741	-111.055	-88.012	10.686
1900	19.862	139.732	123.034	31.727	-111.373	-86.724	9.975
2000	19.863	140.750	123.893	33.714	-111.691	-85.405	9.333

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
1795 K, melting point of Er; ΔH° = 4.757 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.857 + 0.012\times10^{-3}T - 0.351\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.857\times10^{-3}T + 0.006\times10^{-6}T^2 + 0.351\times10^{2}T^{-1} - 6.039$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -79.797 - 4.739\times10^{-3}T - 3.491\times10^{-6}T^2 + 95.400T^{-1}$

$\Delta Gf^\circ = -79.797 + 4.739\times10^{-3}T\ln T + 3.491\times10^{-6}T^2 + 47.700T^{-1} - 77.286\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -81.980 - 14.345\times10^{-3}T - 1.253\times10^{-6}T^2 + 95.400T^{-1}$

$\Delta Gf^\circ = -81.980 + 14.345\times10^{-3}T\ln T + 1.253\times10^{-6}T^2 + 47.700T^{-1} - 128.009\times10^{-3}T$

458.4-1795 K: $\Delta Hf^\circ = -104.049 + 1.165\times10^{-3}T - 1.355\times10^{-6}T^2 + 72.450T^{-1}$

$\Delta Gf^\circ = -104.049 - 1.165\times10^{-3}T\ln T + 1.355\times10^{-6}T^2 + 36.225T^{-1} + 15.186\times10^{-3}T$

1795-2000 K: $\Delta Hf^\circ = -105.703 - 2.804\times10^{-3}T - 0.096\times10^{-6}T^2 + 12.150T^{-1}$

$\Delta Gf^\circ = -105.703 + 2.804\times10^{-3}T\ln T + 0.096\times10^{-6}T^2 + 6.075T^{-1} - 11.370\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166) and Schumm (207). Other data based on Myers (165) and Dieke (56).

$EuBr_2(c,l)$

Europium Dibromide

[Formation: $Eu(c,l) + Br_2(l,g) = EuBr_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	19.700	32.700	32.700	0	-172.000	-165.358	121.209
300	19.700	32.820	32.700	.040	-172.005	-165.311	120.428
332.6	19.830	34.859	32.801	.684	-172.165	-164.576	108.141
332.6	19.830	34.859	32.801	.684	-179.230	-164.576	108.141
400	20.100	38.540	33.465	2.030	-178.922	-161.636	88.312
500	20.500	43.070	34.950	4.060	-178.454	-157.368	68.785
600	20.900	46.840	36.623	6.130	-177.980	-153.192	55.800
700	21.300	50.100	38.329	8.240	-177.501	-149.104	46.552
800	21.700	52.970	39.983	10.390	-177.016	-145.079	39.633
900	22.100	55.550	41.572	12.580	-176.541	-141.117	34.267
956	22.300	56.890	42.436	13.820	-176.287	-138.926	31.759
956	26.000	63.180	42.436	19.830	-170.277	-138.926	31.759
1000	26.000	64.350	43.380	20.970	-169.927	-137.496	30.049
1090	26.000	66.593	45.207	23.310	-169.248	-134.610	26.990
1090	26.000	66.593	45.207	23.310	-171.450	-134.610	26.990
1100	26.000	66.830	45.403	23.570	-171.371	-134.272	26.677
1200	26.000	69.090	47.282	26.170	-170.585	-130.931	23.845
1300	26.000	71.170	49.039	28.770	-169.801	-127.656	21.461
1400	26.000	73.100	50.693	31.370	-169.018	-124.448	19.427
1500	26.000	74.890	52.243	33.970	-168.237	-121.285	17.671

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
956 K, melting point of $EuBr_2$; ΔH° = 6.010 kcal/mol.
1090 K, melting point of Eu; ΔH° = 2.202 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-956 K: $Cp^\circ = 18.500 + 4.000\times10^{-3}T$

$H^\circ - H^\circ_{298} = 18.500\times10^{-3}T + 2.000\times10^{-6}T^2 - 5.694$

956-1500 K: $Cp^\circ = Cp = 26.000$

$H^\circ - H^\circ_{298} = 26.000\times10^{-3}T - 5.026$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -171.109 - 3.887\times10^{-3}T - 0.180\times10^{-6}T^2 + 84.600T^{-1}$

$\Delta Gf^\circ = -171.109 + 3.887\times10^{-3}T\ln T + 0.180\times10^{-6}T^2 + 42.300T^{-1} - 3.386\times10^{-3}T$

332.6-956 K: $\Delta Hf^\circ = -181.109 + 5.274\times10^{-3}T - 0.335\times10^{-6}T^2 + 53.200T^{-1}$

$\Delta Gf^\circ = -181.109 - 5.274\times10^{-3}T\ln T + 0.335\times10^{-6}T^2 + 26.600T^{-1} + 79.969\times10^{-3}T$

956-1090 K: $\Delta Hf^\circ = -180.441 + 12.774\times10^{-3}T - 2.335\times10^{-6}T^2 + 53.200T^{-1}$

$\Delta Gf^\circ = -180.441 - 12.774\times10^{-3}T\ln T + 2.335\times10^{-6}T^2 + 26.600T^{-1} + 128.829\times10^{-3}T$

1090-1500 K: $\Delta Hf^\circ = -180.027 + 7.960\times10^{-3}T - 0.055\times10^{-6}T^2 - 31.400T^{-1}$

$\Delta Gf^\circ = -180.027 - 7.960\times10^{-3}T\ln T + 0.055\times10^{-6}T^2 - 15.700T^{-1} + 97.301\times10^{-3}T$

Source: Data from Haschke (98).

$EuBr_2(g)$

Europium Dibromide (ideal gas)

[Formation: $Eu(c,l) + Br_2(l,g) = EuBr_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	14.500	80.600	80.600	0	-89.000	-96.639	70.837
300	14.500	80.690	80.600	.030	-89.015	-96.682	70.432
332.6	14.555	82.189	80.675	.504	-89.345	-97.499	64.065
332.6	14.555	82.189	80.675	.504	-96.410	-97.499	64.065
400	14.670	84.890	81.175	1.486	-96.466	-97.720	53.391
500	14.750	88.170	82.254	2.958	-96.556	-98.020	42.844
600	14.800	90.870	83.477	4.436	-96.674	-98.304	35.807
700	14.840	93.150	84.699	5.916	-96.825	-98.563	30.772
800	14.890	95.140	85.885	7.404	-97.002	-98.801	26.991
900	14.940	96.890	87.009	8.893	-97.228	-99.010	24.043
1000	15.000	98.470	88.077	10.393	-97.504	-99.193	21.678
1090	15.072	99.772	88.996	11.746	-97.812	-99.340	19.918
1090	15.072	99.772	88.996	11.746	-100.014	-99.340	19.918
1100	15.080	99.910	89.095	11.897	-100.044	-99.333	19.735
1200	15.160	101.220	90.046	13.409	-100.346	-99.248	18.075
1300	15.250	102.440	90.955	14.930	-100.641	-99.147	16.668
1400	15.340	103.570	91.814	16.459	-100.929	-99.017	15.457
1500	15.440	104.630	92.631	17.998	-101.209	-98.867	14.405

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
1090 K, melting point of Eu; $\Delta H°$ = 2.202 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 14.550 + 0.506\times10^{-3}T - 0.179\times10^{5}T^{-2}$

$H°- H°_{298} = 14.550\times10^{-3}T + 0.253\times10^{-6}T^2 + 0.179\times10^{2}T^{-1} - 4.421$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -86.836 - 7.837\times10^{-3}T - 1.927\times10^{-6}T^2 + 102.500T^{-1}$

$\Delta Gf° = -86.836 + 7.837\times10^{-3}T\ln T + 1.927\times10^{-6}T^2 + 51.250T^{-1} - 78.683\times10^{-3}T$

332.6-1090 K: $\Delta Hf° = -96.836 + 1.324\times10^{-3}T - 2.082\times10^{-6}T^2 + 71.100T^{-1}$

$\Delta Gf° = -96.836 - 1.324\times10^{-3}T\ln T + 2.082\times10^{-6}T^2 + 35.550T^{-1} + 4.672\times10^{-3}T$

1090-1500 K: $\Delta Hf° = -96.422 - 3.490\times10^{-3}T + 0.198\times10^{-6}T^2 - 13.500T^{-1}$

$\Delta Gf° = -96.422 + 3.490\times10^{-3}T\ln T - 0.198\times10^{-6}T^2 - 6.750T^{-1} - 26.855\times10^{-3}T$

Source: Data from Haschke (98).

$EuBr_3(c)$

Europium Tribromide

[Formation: $Eu(c) + 1.5Br_2(l,g) = EuBr_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	26.440	43.700	43.700	0	-180.000	-171.214	125.502
300*	26.460	43.864	43.701	.049	-180.012	-171.158	124.687
332.6	26.701	46.606	43.853	.916	-180.244	-170.185	111.826
332.6	26.701	46.606	43.853	.916	-190.841	-170.185	111.826
400	27.200	51.584	44.749	2.734	-190.355	-166.047	90.723
500	27.900	57.736	46.752	5.492	-189.600	-160.056	69.960
600	28.500	62.883	49.021	8.317	-188.816	-154.218	56.173
667	28.850	65.922	50.570	10.240	-188.281	-150.384	49.274

*Data above 298 estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
667 K, $EuBr_3$ vaporizes via $EuBr_3(c) = EuBr_2(c) + Br_2(g)$. Vapor pressure $Br_2(g)$ = 1 atm at 667 K.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-667 K: $Cp^\circ = 25.138 + 5.844\times10^{-3}T - 0.391\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.138\times10^{-3}T + 2.922\times10^{-6}T^2 + 0.391\times10^{2}T^{-1} - 7.886$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -178.609 - 6.294\times10^{-3}T + 0.792\times10^{-6}T^2 + 123.700T^{-1}$

$\Delta Gf^\circ = -178.609 + 6.294\times10^{-3}T\ln T - 0.792\times10^{-6}T^2 + 61.850T^{-1} - 11.521\times10^{-3}T$

332.6-667 K: $\Delta Hf^\circ = -193.609 + 7.447\times10^{-3}T + 0.559\times10^{-6}T^2 + 76.600T^{-1}$

$\Delta Gf^\circ = -193.609 - 7.447\times10^{-3}T\ln T - 0.559\times10^{-6}T^2 + 38.300T\text{-}1 + 113.511\times10^{-3}T$

Sources: Enthalpy of formation at 298 K and vaporization data from Haschke (98). Low-temperature heat capacities and entropy at 298 K from Deline (55). Data above 298 K estimated.

$EuCl_3(c,l)$
Europium Trichloride
[Formation: $Eu(c,l) + 1.5Cl_2(g) = EuCl_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	25.570	34.430	34.430	0	-223.700	-204.587	149.964
300*	25.590	34.588	34.431	.047	-223.688	-204.469	148.953
400	26.600	42.102	35.447	2.662	-222.982	-198.165	108.271
500	27.400	48.125	37.401	5.362	-222.242	-192.044	83.941
600	28.100	53.179	39.621	8.135	-221.480	-186.075	67.777
700	28.800	57.562	41.878	10.979	-220.691	-180.236	56.271
800	29.500	61.450	44.085	13.892	-219.878	-174.512	47.674
897	30.100	64.857	46.150	16.780	-219.075	-169.057	41.189
897	34.000	78.458	46.150	28.980	-206.875	-169.057	41.189
900	34.000	78.571	46.258	29.082	-206.839	-168.930	41.021
1000	34.000	82.154	49.672	32.482	-205.656	-164.784	36.013
1090	34.000	85.083	52.476	35.542	-204.655	-161.149	32.311
1090	34.000	85.083	52.476	35.542	-206.857	-161.149	32.311
1100	34.000	85.394	52.774	35.882	-206.743	-160.731	31.934
1200	34.000	88.353	55.618	39.282	-205.604	-156.598	28.520
1300	34.000	91.074	58.242	42.682	-204.468	-152.559	25.647

*Data above 298 K except temperature and enthalpy of fusion estimated.

Phase changes: 897 K, melting point of $EuCl_3$; ΔH° = 12.200 kcal/mol.
1090 K, melting point of Eu; ΔH° = 2.202 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-897 K: $Cp^\circ = 24.583 + 6.238\times10^{-3}T - 0.776\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 24.583\times10^{-3}T + 3.119\times10^{-6}T^2 + 0.776\times10^{2}T^{-1} - 7.867$

897-1300 K: $Cp^\circ = 34.000$
$H^\circ - H^\circ_{298} = 34.000\times10^{-3}T - 1.518$

Formation equations (kcal/mol):

298.15-897 K: $\Delta Hf^\circ = -226.064 + 7.047\times10^{-3}T + 0.707\times10^{-6}T^2 + 59.750T^{-1}$
$\Delta Gf^\circ = -226.064 - 7.047\times10^{-3}T\ln T - 0.707\times10^{-6}T^2 + 29.875T^{-1} + 112.057\times10^{-3}T$

897-1090 K: $\Delta Hf^\circ = -219.715 + 16.464\times10^{-3}T - 2.412\times10^{-6}T^2 - 17.850T^{-1}$
$\Delta Gf^\circ = -219.715 - 16.464\times10^{-3}T\ln T + 2.412\times10^{-6}T^2 - 8.925T^{-1} + 166.256\times10^{-3}T$

1090-1300 K: $\Delta Hf^\circ = -219.301 + 11.650\times10^{-3}T - 0.132\times10^{-6}T^2 - 102.450T^{-1}$
$\Delta Gf^\circ = -219.301 - 11.650\times10^{-3}T\ln T + 0.132\times10^{-6}T^2 - 51.225T^{-1} + 134.729\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (207). Low-temperature heat capacities and entropy at 298 K from Sommers (220). Temperature and enthalpy of fusion from Kulagin (137). Other high-temperature data estimated.

$EuCl_3(g)$

Europium Trichloride (ideal gas)

[Formation: $Eu(c,l,g) + 1.5Cl_2(g) = EuCl_3(g)$

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	21.030	86.894	86.894	0	-157.300	-153.829	112.758
300	21.043	87.024	86.894	.039	-157.296	-153.807	112.047
400	21.523	93.151	87.726	2.170	-157.075	-152.676	83.417
500	21.790	97.985	89.311	4.337	-156.867	-151.599	66.263
600	21.959	101.974	91.099	6.525	-156.691	-150.562	54.841
700	22.077	105.368	92.901	8.727	-156.544	-149.552	46.692
800	22.161	108.322	94.648	10.939	-156.431	-148.563	40.585
900	22.216	110.936	96.316	13.158	-156.363	-147.583	35.837
1000	22.244	113.278	97.897	15.381	-156.357	-146.609	32.041
1090	22.244	115.195	99.247	17.384	-156.414	-145.729	29.219
1090	22.244	115.195	99.247	17.384	-158.616	-145.729	29.219
1100	22.244	115.398	99.393	17.606	-158.619	-145.611	28.930
1200	22.220	117.333	100.809	19.829	-158.657	-144.427	26.303
1300	22.175	119.110	102.149	22.049	-158.701	-143.239	24.080
1400	22.112	120.751	103.420	24.264	-158.753	-142.047	22.174
1500	22.036	122.274	104.627	26.471	-158.816	-140.851	20.522
1600	21.951	123.694	105.775	28.671	-158.889	-139.651	19.075
1700	21.861	125.022	106.868	30.861	-158.974	-138.445	17.798
1800	21.768	126.269	107.912	33.043	-159.069	-137.239	16.663
1800	21.768	126.269	107.912	33.043	-193.654	-137.239	16.663
1900	21.674	127.443	108.909	35.215	-193.353	-134.106	15.426
2000	21.581	128.552	109.863	37.378	-193.070	-130.995	14.314

Phase changes: 1090 K, melting point of Eu; ΔH° = 2.202 kcal/mol.
1800 K, boiling point of Eu; ΔH° = 34.585 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 22.598 - 0.350\times10^{-3}T - 1.301\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 22.598\times10^{-3}T - 0.175\times10^{-6}T^2 + 1.301\times10^{2}T^{-1} - 7.158$

Formation equations (kcal/mol):

298.15-1090 K: $\Delta Hf^\circ = -158.956 + 5.061\times10^{-3}T - 2.587\times10^{-6}T^2 + 112.250T^{-1}$

$\Delta Gf^\circ = -158.956 - 5.061\times10^{-3}T\ln T + 2.587\times10^{-6}T^2 + 56.125T^{-1} + 44.630\times10^{-3}T$

1090-1800 K: $\Delta Hf^\circ = -158.542 + 0.248\times10^{-3}T - 0.307\times10^{-6}T^2 + 27.650T^{-1}$

$\Delta Gf^\circ = -158.542 - 0.248\times10^{-3}T\ln T + 0.307\times10^{-6}T^2 + 13.825T^{-1} + 13.102\times10^{-3}T$

1800-2000 K: $\Delta Hf^\circ = -201.354 + 5.278\times10^{-3}T - 0.562\times10^{-6}T^2 + 27.650T^{-1}$

$\Delta Gf^\circ = -201.354 - 5.278\times10^{-3}T\ln T + 0.562\times10^{-6}T^2 + 13.825T^{-1} + 74.130\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

$EuF_3(c)$
Europium Trifluoride
[Formation: $Eu(c,l) + 1.5F_2(g) = EuF_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	23.800	25.600	25.600	0	-378.600	-359.022	263.167
300	23.830	25.747	25.600	.044	-378.589	-358.901	261.456
400	24.994	32.777	26.552	2.490	-377.962	-352.429	192.556
500	25.818	38.445	28.381	5.032	-377.305	-346.119	151.287
600	26.596	43.221	30.466	7.653	-376.638	-339.944	123.823
700	27.430	47.382	32.592	10.353	-375.948	-333.882	104.241
800	28.362	51.105	34.678	13.142	-375.221	-327.923	89.583
900	29.411	54.505	36.694	16.030	-374.456	-322.054	78.204
920	29.636	55.152	37.088	16.620	-374.299	-320.891	76.228
920	36.000	56.817	37.088	18.150	-372.769	-320.891	76.228
1000	36.000	59.818	38.788	21.030	-371.652	-316.429	69.155
1090	36.000	62.920	40.654	24.270	-370.457	-311.511	62.458
1090	36.000	62.920	40.654	24.270	-372.659	-311.511	62.458
1100	36.000	63.249	40.858	24.630	-372.523	-310.951	61.779
1200	36.000	66.382	42.857	28.230	-371.171	-305.414	55.623
1300	36.000	69.263	44.778	31.830	-369.824	-299.985	50.431
1400	36.000	71.931	46.624	35.430	-368.485	-294.666	45.999
1500	36.000	74.415	48.395	39.030	-367.151	-289.439	42.171

*Entropy and heat capacity at 298 K estimated.

Phase changes: 920 K α - β transition point of EuF_3; ΔH° = 1.530 kcal/mol.
1090 K, melting point of Eu; ΔH° = 2.202 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-920 K: $Cp^\circ = 22.246 + 7.760\times10^{-3}T - 0.676\times10^{5}T^{-2}$.

$H^\circ - H^\circ_{298} = 22.246\times10^{-3}T + 3.880\times10^{-6}T^2 + 0.676\times10^{2}T^{-1} - 7.204$

920-1500 K: $Cp^\circ = 36.000$

$H^\circ - H^\circ_{298} = 36.000\times10^{-3}T - 14.970$

Formation equations (kcal/mol):

298.15-920 K: $\Delta Hf^\circ = -380.271 + 5.188\times10^{-3}T + 1.339\times10^{-6}T^2 + 1.450T^{-1}$

$\Delta Gf^\circ = -380.271 - 5.188\times10^{-3}T\ln T - 1.339\times10^{-6}T^2 + 0.725T^{-1} + 101.218\times10^{-3}T$

920-1090 K: $\Delta Hf^\circ = -388.037 + 18.942\times10^{-3}T - 2.541\times10^{-6}T^2 - 66.150T^{-1}$

$\Delta Gf^\circ = -388.037 - 18.942\times10^{-3}T\ln T + 2.541\times10^{-6}T^2 - 33.075T^{-1} + 199.992\times10^{-3}T$

1090-1500 K: $\Delta Hf^\circ = -387.623 + 14.128\times10^{-3}T - 0.261\times10^{-6}T^2 - 150.750T^{-1}$

$\Delta Gf^\circ = -387.623 - 14.128\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 - 75.375T^{-1} + 168.465\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Kim (122). High-temperature data based on Spedding (222). Entropy and heat capacity at 298 K estimated.

$EuF_3(g)$

Europium Trifluoride (ideal gas)

[Formation: $Eu(c,l,g) + 1.5F_2(g) = EuF_3(g)$

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.482	78.459	78.459	0	-274.300	-270.482	198.266
300	19.506	78.580	78.460	.036	-274.297	-270.459	197.026
400	20.489	84.339	79.239	2.040	-274.111	-269.203	147.084
500	21.068	88.979	80.737	4.121	-273.916	-267.997	117.140
600	21.433	92.854	82.442	6.247	-273.743	-266.830	97.191
700	21.679	96.178	84.174	8.403	-273.598	-265.690	82.951
800	21.850	99.085	85.860	10.580	-273.483	-264.569	72.276
900	21.967	101.666	87.475	12.772	-273.414	-263.457	63.975
1000	22.040	103.984	89.012	14.972	-273.410	-262.353	57.336
1090	22.072	105.885	90.328	16.957	-273.469	-261.356	52.402
1090	22.072	105.885	90.328	16.957	-275.671	-261.356	52.402
1100	22.075	106.087	90.471	17.178	-275.675	-261.224	51.900
1200	22.077	108.008	91.853	19.386	-275.714	-259.909	47.335
1300	22.053	109.774	93.164	21.593	-275.761	-258.587	43.472
1400	22.006	111.407	94.410	23.796	-275.819	-257.266	40.161
1500	21.944	112.923	95.594	25.994	-275.886	-255.937	37.290
1600	21.870	114.337	96.722	28.184	-275.966	-254.605	34.777
1700	21.789	115.660	97.797	30.367	-276.056	-253.265	32.559
1800	21.703	116.903	98.824	32.542	-276.160	-251.925	30.587
1800	21.703	116.903	98.824	32.542	-310.745	-251.925	30.587
1900	21.616	118.074	99.807	34.708	-310.452	-248.660	28.602
2000	21.529	119.181	100.748	36.865	-310.177	-245.417	26.818

Phase changes: 1090 K, melting point of Eu; $\Delta H°$ = 2.202 kcal/mol.
1800 K, boiling point of Eu; $\Delta H°$ = 34.585 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 22.294 - 0.176\times10^{-3}T - 2.453\times10^{5}T^{-2}$

$H°- H°_{298} = 22.294\times10^{-3}T - 0.088\times10^{-6}T^{2} + 2.453\times10^{2}T^{-1} - 7.462$

Formation equations (kcal/mol):

298.15-1090 K: $\Delta Hf° = -276.228 + 5.236\times10^{-3}T - 2.629\times10^{-6}T^{2} + 179.150T^{-1}$

$\Delta Gf° = -276.228 - 5.236\times10^{-3}T\ln T + 2.629\times10^{-6}T^{2} + 89.575T^{-1} + 47.314\times10^{-3}T$

1090-1800 K: $\Delta Hf° = -275.814 + 0.422\times10^{-3}T - 0.349\times10^{-6}T^{2} + 94.550T^{-1}$

$\Delta Gf° = -275.814 - 0.422\times10^{-3}T\ln T + 0.349\times10^{-6}T^{2} + 47.275T^{-1} + 15.786\times10^{-3}T$

1800-2000 K: $\Delta Hf° = -318.627 + 5.452\times10^{-3}T - 0.604\times10^{-6}T^{2} + 94.550T^{-1}$

$\Delta Gf° = -318.627 - 5.452\times10^{-3}T\ln T + 0.604\times10^{-6}T^{2} + 47.275T^{-1} + 76.815\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

$FeBr_2$(c,l)
Iron Dibromide
[Formation: Fe(c) + Br_2(l,g) = $FeBr_2$(c,l)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.176	33.620	33.620	0	-59.500	-56.733	41.586
300	19.186	33.739	33.622	.035	-59.509	-56.716	41.317
332.6	19.359	35.727	33.733	.663	-59.667	-56.405	37.063
332.6	19.359	35.727	33.733	.663	-66.732	-56.405	37.063
400	19.718	39.331	34.379	1.981	-66.431	-54.343	29.691
500	20.250	43.788	35.830	3.979	-65.997	-51.372	22.455
600	20.782	47.527	37.475	6.031	-65.570	-48.486	17.661
650	21.048	49.201	38.315	7.076	-65.360	-47.072	15.827
650	21.048	49.355	38.315	7.176	-65.260	-47.072	15.827
700	21.314	50.924	39.160	8.235	-65.054	-45.680	14.262
800	21.846	53.805	40.814	10.393	-64.656	-42.940	11.731
900	22.378	56.409	42.403	12.605	-64.305	-40.247	9.773
964	22.719	57.959	43.386	14.048	-64.125	-38.545	8.738
964*	25.500	70.407	43.386	26.048	-52.125	-38.545	8.738
1000	25.500	71.342	44.376	26.966	-51.980	-38.040	8.314
1043	25.500	72.416	45.510	28.063	-51.905	-37.443	7.846
1100	25.500	73.772	46.939	29.516	-51.664	-36.657	7.283
1185	25.500	75.670	48.933	31.684	-51.148	-35.516	6.550
1185	25.500	75.670	48.933	31.684	-51.363	-35.516	6.550
1200	25.500	75.991	49.269	32.066	-51.238	-35.318	6.432
1207	25.500	76.139	49.425	32.244	-51.180	-35.225	6.378

*Enthalpy of fusion and heat capacity of liquid estimated.

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
650 K, α - β transition point of $FeBr_2$; $\Delta H°$ = 0.100 kcal/mol.
964 K, melting point of $FeBr_2$; $\Delta H°$ = 12.000 kcal/mol.
1043 K, Curie temperature of Fe; $\Delta H°$ = 0 kcal/mol.
1185 K, α - γ transition point of Fe; $\Delta H°$ = 0.215 kcal/mol.
1207 K, boiling point of $FeBr_2$ to equilibrium mixture of monomer and dimer; $\Delta H°$ = 29.4 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-650 K: $Cp° = 17.590 + 5.318\times10^{-3}T$
$H°- H°_{298} = 17.590\times10^{-3}T + 2.659\times10^{-6}T^2 - 5.481$

650-964 K: $Cp° = 17.590 + 5.320\times10^{-3}T$
$H°- H°_{298} = 17.590\times10^{-3}T + 2.660\times10^{-6}T^2 - 5.381$

964-1207 K: $Cp° = 25.500$
$H°- H°_{298} = 25.500\times10^{-3}T + 1.466$

$FeBr_2$(c,l) - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -59.888 - 0.280\times10^{-3}T - 3.312\times10^{-6}T^2 + 228.500T^{-1}$

$\Delta Gf^\circ = -59.888 + 0.280\times10^{-3}T\ln T + 3.312\times10^{-6}T^2 + 114.250T^{-1} + 6.714\times10^{-3}T$

332.6-650 K: $\Delta Hf^\circ = -69.889 + 8.881\times10^{-3}T - 3.467\times10^{-6}T^2 + 197.100T^{-1}$

$\Delta Gf^\circ = -69.889 - 8.881\times10^{-3}T\ln T + 3.467\times10^{-6}T^2 + 98.550T^{-1} + 90.069\times10^{-3}T$

650-964 K: $\Delta Hf^\circ = -69.789 + 8.881\times10^{-3}T - 3.466\times10^{-6}T^2 + 197.100T^{-1}$

$\Delta Gf^\circ = -69.789 - 8.881\times10^{-3}T\ln T + 3.466\times10^{-6}T^2 + 98.550T^{-1} + 89.917\times10^{-3}T$

964-1043 K: $\Delta Hf^\circ = -62.943 + 16.791\times10^{-3}T - 6.126\times10^{-6}T^2 + 197.100T^{-1}$

$\Delta Gf^\circ = -62.943 - 16.791\times10^{-3}T\ln T + 6.126\times10^{-6}T^2 + 98.550T^{-1} + 134.600\times10^{-3}T$

1043-1185 K: $\Delta Hf^\circ = -39.382 - 27.190\times10^{-3}T + 14.585\times10^{-6}T^2 - 31.400T^{-1}$

$\Delta Gf^\circ = -39.382 + 27.190\times10^{-3}T\ln T - 14.585\times10^{-6}T^2 - 15.700T^{-1} - 171.944\times10^{-3}T$

1185-1207 K: $\Delta Hf^\circ = -62.996 + 11.065\times10^{-3}T - 1.106\times10^{-6}T^2 + 87.600T^{-1}$

$\Delta Gf^\circ = -62.996 - 11.065\times10^{-3}T\ln T + 1.106\times10^{-6}T^2 + 43.800T^{-1} + 100.097\times10^{-3}T$

Source: Data from JANAF (60) who estimated enthalpy of fusion and heat capacity of liquid.

$FeBr_2(g)$
Iron Dibromide (ideal gas)
[Formation: $Fe(c,l) + Br_2(l,g) = FeBr_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	14.496	80.604	80.604	0	-9.900	-21.142	15.497
300	14.501	80.693	80.604	.027	-9.917	-21.210	15.452
332.6	14.556	82.192	80.687	.501	-10.229	-22.422	14.733
332.6	14.556	82.192	80.687	.501	-17.294	-22.422	14.733
400	14.669	84.891	81.176	1.486	-17.326	-23.462	12.819
500	14.752	88.174	82.258	2.958	-17.418	-24.986	10.921
600	14.802	90.869	83.476	4.436	-17.565	-26.486	9.648
700	14.842	93.153	84.699	5.918	-17.771	-27.957	8.729
800	14.886	95.138	85.883	7.404	-18.045	-29.395	8.030
900	14.939	96.894	87.011	8.895	-18.415	-30.794	7.478
1000	15.004	98.472	88.079	10.393	-18.953	-32.143	7.025
1043	15.037	99.104	88.521	11.039	-19.329	-32.703	6.852
1100	15.080	99.905	89.090	11.897	-19.683	-33.422	6.640
1185	15.151	101.030	89.907	13.182	-20.050	-34.470	6.357
1185	15.151	101.030	89.907	13.182	-20.265	-34.470	6.357
1200	15.164	101.221	90.047	13.409	-20.295	-34.651	6.311
1300	15.253	102.438	90.953	14.930	-20.499	-35.838	6.025
1400	15.344	103.572	91.816	16.459	-20.717	-37.010	5.777
1500	15.435	104.633	92.634	17.998	-20.947	-38.166	5.561
1600	15.523	105.632	93.416	19.546	-21.189	-39.304	5.369
1667	15.579	106.270	93.920	20.588	-21.358	-40.061	5.252
1667	15.579	106.270	93.920	20.588	-21.558	-40.061	5.252
1700	15.606	106.576	94.162	21.103	-21.669	-40.427	5.197
1800	15.682	107.470	94.877	22.667	-22.016	-41.519	5.041
1811	15.690	107.566	94.954	22.840	-22.059	-41.641	5.025
1811	15.690	107.566	94.954	22.840	-25.359	-41.641	5.025
1900	15.751	108.320	95.563	24.239	-25.750	-42.430	4.881
2000	15.812	109.129	96.220	25.817	-26.186	-43.298	4.731

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
1043 K, Curie temperature of Fe; $\Delta H°$ = 0 kcal/mol.
1185 K, α - γ transition point of Fe; $\Delta H°$ = 0.215 kcal/mol.
1667 K, γ - δ transition point of Fe; $\Delta H°$ = 0.200 kcal/mol.
1811 K, melting point of Fe; $\Delta H°$ = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 14.435 + 0.648\times10^{-3}T - 0.118\times10^{5}T^{-2}$

$H°- H°_{298} = 14.435\times10^{-3}T + 0.324\times10^{-6}T^{2} + 0.118\times10^{2}T^{-1} - 4.372$

$FeBr_2(g)$ - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -9.180 - 3.435\times10^{-3}T - 5.647\times10^{-6}T^2 + 240.300T^{-1}$

$\Delta Gf^\circ = -9.180 + 3.435\times10^{-3}T\ln T + 5.647\times10^{-6}T^2 + 120.150T^{-1} - 62.727\times10^{-3}T$

332.6-1043 K: $\Delta Hf^\circ = -19.180 + 5.726\times10^{-3}T - 5.802\times10^{-6}T^2 + 208.900T^{-1}$

$\Delta Gf^\circ = -19.180 - 5.726\times10^{-3}T\ln T + 5.802\times10^{-6}T^2 + 104.450T^{-1} + 20.628\times10^{-3}T$

1043-1185 K: $\Delta Hf^\circ = 4.381 - 38.255\times10^{-3}T + 14.909\times10^{-6}T^2 - 19.600T^{-1}$

$\Delta Gf^\circ = 4.381 + 38.255\times10^{-3}T\ln T - 14.909\times10^{-6}T^2 - 9.800T^{-1} - 285.916\times10^{-3}T$

1185-1667 K: $\Delta Hf^\circ = -19.233 - 0.782\times10^{-6}T^2 + 99.400T^{-1}$

$\Delta Gf^\circ = -19.233 + 0.782\times10^{-6}T^2 + 49.700T^{-1} - 13.876\times10^{-3}T$

1667-1811 K: $\Delta Hf^\circ = -102.128 + 48.497\times10^{-3}T - 10.413\times10^{-6}T^2 + 47798.600T^{-1}$

$\Delta Gf^\circ = -102.128 - 48.497\times10^{-3}T\ln T + 10.413\times10^{-6}T^2 + 23899.301T^{-1} + 371.003\times10^{-3}T$

1811-2000 K: $\Delta Hf^\circ = -16.278 - 5.495\times10^{-3}T + 0.269\times10^{-6}T^2 - 19.600T^{-1}$

$\Delta Gf^\circ = -16.278 + 5.495\times10^{-3}T\ln T - 0.269\times10^{-6}T^2 - 9.800T^{-1} - 54.795\times10^{-3}T$

Source: Data from JANAF (60) who estimated molecular constants.

$(FeBr_2)_2(g)$

Dimeric Iron Dibromide (ideal gas)

[Formation: $2Fe(c,l) + 2Br_2(l,g) = (FeBr_2)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	31.234	123.304	123.304	0	-60.500	-71.682	52.544
300	31.240	123.497	123.304	.058	-60.530	-71.750	52.269
332.6	31.318	126.724	123.483	1.078	-61.082	-72.942	47.929
332.6	31.318	126.724	123.483	1.078	-75.212	-72.942	47.929
400	31.479	132.522	124.535	3.195	-75.129	-72.497	39.610
500	31.593	139.560	126.860	6.350	-75.102	-71.845	31.403
600	31.659	145.326	129.473	9.512	-75.190	-71.186	25.929
700	31.709	150.210	132.094	12.681	-75.397	-70.503	22.012
800	31.759	154.447	134.630	15.854	-75.744	-69.782	19.063
900	31.817	158.191	137.043	19.033	-76.287	-69.007	16.757
1000	31.888	161.547	139.329	22.218	-77.174	-68.157	14.896
1043	31.923	162.890	140.273	23.590	-77.845	-67.757	14.198
1100	31.970	164.590	141.489	25.411	-78.449	-67.185	13.348
1185	32.049	166.973	143.233	28.131	-79.032	-66.293	12.226
1185	32.049	166.973	143.233	28.131	-79.462	-66.293	12.226
1200	32.063	167.376	143.533	28.612	-79.496	-66.128	12.043
1300	32.164	169.946	145.466	31.824	-79.734	-65.002	10.928
1400	32.270	172.333	147.301	35.045	-80.007	-63.858	9.969
1500	32.377	174.563	149.044	38.278	-80.312	-62.695	9.134
1600	32.482	176.656	150.705	41.521	-80.649	-61.507	8.401
1667	32.550	177.991	151.776	43.699	-80.894	-60.706	7.959
1667	32.550	177.991	151.776	43.699	-81.294	-60.706	7.959
1700	32.584	178.629	152.291	44.774	-81.470	-60.297	7.752
1800	32.681	180.494	153.807	48.037	-82.029	-59.032	7.167
1811	32.691	180.693	153.969	48.397	-82.100	-58.898	7.108
1811	32.691	180.693	153.969	48.397	-88.700	-58.898	7.108
1900	32.770	182.263	155.258	51.310	-89.368	-57.412	6.604
2000	32.850	183.946	156.650	54.591	-90.115	-55.715	6.088

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.
1667 K, γ - δ transition point of Fe; ΔH° = 0.200 kcal/mol.
1811 K, melting point of Fe; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 31.291 + 0.704\times10^{-3}T - 0.237\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 31.291\times10^{-3}T + 0.352\times10^{-6}T^2 + 0.237\times10^{2}T^{-1} - 9.440$

$(FeBr_2)_2(g)$ - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -59.756 - 4.449\times10^{-3}T - 11.590\times10^{-6}T^2 + 480.700T^{-1}$

$\Delta Gf^\circ = -59.756 + 4.449\times10^{-3}T\ln T + 11.590\times10^{-6}T^2 + 240.350T^{-1} - 71.511\times10^{-3}T$

332.6-1043 K: $\Delta Hf^\circ = -79.756 + 13.873\times10^{-3}T - 11.900\times10^{-6}T^2 + 417.900T^{-1}$

$\Delta Gf^\circ = -79.756 - 13.873\times10^{-3}T\ln T + 11.900\times10^{-6}T^2 + 208.950T^{-1} + 95.199\times10^{-3}T$

1043-1185 K: $\Delta Hf^\circ = -32.635 - 74.089\times10^{-3}T + 29.522\times10^{-6}T^2 - 39.100T^{-1}$

$\Delta Gf^\circ = -32.635 + 74.089\times10^{-3}T\ln T - 29.522\times10^{-6}T^2 - 19.550T^{-1} - 517.890\times10^{-3}T$

1185-1667 K: $\Delta Hf^\circ = -79.862 + 2.421\times10^{-3}T - 1.860\times10^{-6}T^2 + 198.900T^{-1}$

$\Delta Gf^\circ = -79.862 - 2.421\times10^{-3}T\ln T + 1.860\times10^{-6}T^2 + 99.450T^{-1} + 26.192\times10^{-3}T$

1667-1811 K: $\Delta Hf^\circ = -245.652 + 99.415\times10^{-3}T - 21.122\times10^{-6}T^2 + 95597.300T^{-1}$

$\Delta Gf^\circ = -245.652 - 99.415\times10^{-3}T\ln T + 21.122\times10^{-6}T^2 + 47798.650T^{-1} + 795.948\times10^{-3}T$

1811-2000 K: $\Delta Hf^\circ = -73.952 - 8.569\times10^{-3}T + 0.242\times10^{-6}T^2 - 39.100T^{-1}$

$\Delta Gf^\circ = -73.952 + 8.569\times10^{-3}T\ln T - 0.242\times10^{-6}T^2 - 19.550T^{-1} - 55.647\times10^{-3}T$

Source: Data from JANAF (60) who estimated molecular constants.

FeCl(g)
Iron Monochloride (ideal gas)
[Formation: $Fe(c,l) + 0.5Cl_2(g) = FeCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	9.136	61.537	61.537	0	60.000	51.541	-37.780
300	9.141	61.593	61.537	.017	59.998	51.489	-37.509
400	9.366	64.257	61.900	.943	59.883	48.667	-26.590
500	9.478	66.361	62.589	1.886	59.718	45.881	-20.054
600	9.516	68.093	63.366	2.836	59.496	43.134	-15.711
700	9.520	69.560	64.149	3.788	59.215	40.429	-12.622
800	9.515	70.831	64.906	4.740	58.858	37.768	-10.318
900	9.512	71.952	65.629	5.691	58.403	35.158	-8.537
1000	9.514	72.954	66.311	6.643	57.771	32.606	-7.126
1043	9.517	73.355	66.593	7.052	57.354	31.532	-6.607
1100	9.522	73.861	66.956	7.595	56.943	30.134	-5.987
1185	9.530	74.570	67.478	8.404	56.486	28.080	-5.179
1185	9.530	74.570	67.478	8.404	56.271	28.080	-5.179
1200	9.532	74.690	67.568	8.547	56.224	27.722	-5.049
1300	9.545	75.453	68.145	9.501	55.907	25.361	-4.263
1400	9.559	76.161	68.692	10.456	55.569	23.023	-3.594
1500	9.572	76.821	69.212	11.413	55.212	20.711	-3.018
1600	9.584	77.439	69.707	12.371	54.835	18.425	-2.517
1667	9.591	77.833	70.026	13.013	54.571	16.904	-2.216
1667	9.591	77.833	70.026	13.013	54.371	16.904	-2.216
1700	9.595	78.021	70.180	13.330	54.213	16.164	-2.078
1800	9.605	78.569	70.630	14.290	53.717	13.942	-1.693
1811	9.606	78.628	70.679	14.396	53.658	13.696	-1.653
1811	9.606	78.628	70.679	14.396	50.358	13.696	-1.653
1900	9.612	79.089	71.062	15.251	49.828	11.907	-1.370
2000	9.619	79.582	71.476	16.212	49.231	9.925	-1.085

Phase changes: 1043 K, Curie temperature of Fe; $\Delta H°$ = 0 kcal/mol.
1185 K, α - γ transition point of Fe; $\Delta H°$ = 0.215 kcal/mol.
1667 K, γ - δ transition point of Fe; $\Delta H°$ = 0.200 kcal/mol.
1811 K, melting point of Fe; $\Delta H°$ = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 9.654 - 0.054\times10^{-3}T - 0.447\times10^{5}T^{-2}$

$H°- H°_{298} = 9.654\times10^{-3}T - 0.027\times10^{-6}T^{2} + 0.447\times10^{2}T^{-1} - 3.026$

FeCl(g) - Continued

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf^\circ = 58.116 + 5.462\times10^{-3}T - 6.142\times10^{-6}T^2 + 239.050T^{-1}$

$\Delta Gf^\circ = 58.116 - 5.462\times10^{-3}T\ln T + 6.142\times10^{-6}T^2 + 119.525T^{-1} + 5.889\times10^{-3}T$

1043-1185 K: $\Delta Hf^\circ = 81.677 - 38.519\times10^{-3}T + 14.569\times10^{-6}T^2 + 10.550T^{-1}$

$\Delta Gf^\circ = 81.677 + 38.519\times10^{-3}T\ln T - 14.569\times10^{-6}T^2 + 5.275T^{-1} - 300.655\times10^{-3}T$

1185-1667 K: $\Delta Hf^\circ = 58.063 - 0.265\times10^{-3}T - 1.122\times10^{-6}T^2 + 129.550T^{-1}$

$\Delta Gf^\circ = 58.063 + 0.265\times10^{-3}T\ln T + 1.122\times10^{-6}T^2 + 64.775T^{-1} - 28.615\times10^{-3}T$

1667-1811 K: $\Delta Hf^\circ = -24.832 + 48.232\times10^{-3}T - 10.753\times10^{-6}T^2 + 47828.750T^{-1}$

$\Delta Gf^\circ = -24.832 - 48.232\times10^{-3}T\ln T + 10.753\times10^{-6}T^2 + 23914.375T^{-1} + 356.264\times10^{-3}T$

1811-2000 K: $\Delta Hf^\circ = 61.018 - 5.760\times10^{-3}T - 0.071\times10^{-6}T^2 + 10.550T^{-1}$

$\Delta Gf^\circ = 61.018 + 5.760\times10^{-3}T\ln T + 0.071\times10^{-6}T^2 + 5.275T^{-1} - 69.534\times10^{-3}T$

Source: Data from JANAF (60) who estimated some molecular constants.

$FeCl_2(c,l)$
Iron Dichloride
[Formation: $Fe(c) + Cl_2(g) = FeCl_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	18.290	28.190	28.190	0	-81.650	-72.222	52.940
300	18.309	28.303	28.190	.034	-81.642	-72.164	52.571
400	19.039	33.681	28.919	1.905	-81.227	-69.068	37.736
500	19.493	37.981	30.315	3.833	-80.834	-66.073	28.880
600	19.846	41.567	31.900	5.800	-80.473	-63.156	23.004
700	20.156	44.650	33.506	7.801	-80.145	-60.295	18.825
800	20.448	47.361	35.072	9.831	-79.866	-57.481	15.703
900	20.735	49.786	36.575	11.890	-79.659	-54.696	13.282
950	20.878	50.911	37.300	12.930	-79.588	-53.312	12.264
950	24.400	61.721	37.300	23.200	-69.318	-53.312	12.264
1000	24.400	62.972	38.552	24.420	-69.159	-52.473	11.468
1043	24.400	63.999	39.580	25.469	-69.129	-51.757	10.845
1100	24.400	65.298	40.880	26.860	-68.948	-50.811	10.095
1185	24.400	67.114	42.697	28.934	-68.523	-49.425	9.115
1185	24.400	67.114	42.697	28.934	-68.738	-49.425	9.115
1200	24.400	67.421	43.004	29.300	-68.629	-49.183	8.957
1297	24.400	69.318	44.902	31.667	-67.932	-47.638	8.027

Phase changes: 950 K, melting point of $FeCl_2$; ΔH° = 10.270 kcal/mol.
1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1185 K, $\alpha - \gamma$ transition point of Fe; ΔH° = 0.215 kcal/mol.
1297 K, boiling point of $FeCl_2$ to equilibrium mixture of $FeCl_2(g)$ and $(FeCl_2)_2(g)$; ΔH° = 26.3 kcal/mol of $FeCl_2$.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-950 K: $Cp^\circ = 18.705 + 2.378\times10^{-3}T - 0.999\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 18.705\times10^{-3}T + 1.189\times10^{-6}T^2 + 0.999\times10^{2}T^{-1} - 6.018$

950-1297 K: $Cp^\circ = 24.400$

$H^\circ - H^\circ_{298} = 24.400\times10^{-3}T + 0.020$

Formation equations (kcal/mol):

298.15-950 K: $\Delta Hf^\circ = -85.092 + 10.099\times10^{-3}T - 4.970\times10^{-6}T^2 + 260.100T^{-1}$

$\Delta Gf^\circ = -85.092 - 10.099\times10^{-3}T\ln T + 4.970\times10^{-6}T^2 + 130.050T^{-1} + 97.758\times10^{-3}T$

950-1043 K: $\Delta Hf^\circ = -79.054 + 15.794\times10^{-3}T - 6.159\times10^{-6}T^2 + 160.200T^{-1}$

$\Delta Gf^\circ = -79.054 - 15.794\times10^{-3}T\ln T + 6.159\times10^{-6}T^2 + 80.100T^{-1} + 129.376\times10^{-3}T$

1043-1185 K: $\Delta Hf^\circ = -55.493 - 28.187\times10^{-3}T + 14.552\times10^{-6}T^2 - 68.300T^{-1}$

$\Delta Gf^\circ = -55.493 + 28.187\times10^{-3}T\ln T - 14.552\times10^{-6}T^2 - 34.150T^{-1} - 177.168\times10^{-3}T$

1185-1297 K: $\Delta Hf^\circ = -79.107 + 10.068\times10^{-3}T - 1.139\times10^{-6}T^2 + 50.700T^{-1}$

$\Delta Gf^\circ = -79.107 - 10.068\times10^{-3}T\ln T + 1.139\times10^{-6}T^2 + 25.350T^{-1} + 94.872\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Parker (188). Low-temperature heat capacities from Kelley (119). High-temperature data based on Moore (160). Vaporization data from Chase (25).

$FeCl_2(g)$

Iron Dichloride (ideal gas)

[Formation: $Fe(c,l) + Cl_2(g) = FeCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	13.759	71.503	71.503	0	-33.700	-37.186	27.258
300	13.771	71.588	71.505	.025	-33.701	-37.208	27.106
400	14.210	75.617	72.049	1.427	-33.755	-38.370	20.964
500	14.442	78.816	73.094	2.861	-33.856	-39.513	17.271
600	14.579	81.462	74.275	4.312	-34.011	-40.631	14.800
700	14.673	83.716	75.466	5.775	-34.221	-41.717	13.025
800	14.750	85.681	76.623	7.246	-34.501	-42.772	11.685
900	14.823	87.422	77.728	8.725	-34.874	-43.783	10.632
1000	14.901	88.988	78.777	10.211	-35.418	-44.748	9.780
1043	14.937	89.616	79.211	10.853	-35.796	-45.142	9.459
1100	14.984	90.412	79.771	11.705	-36.153	-45.642	9.068
1185	15.060	91.530	80.575	12.982	-36.525	-46.361	8.550
1185	15.060	91.530	80.575	12.982	-36.740	-46.361	8.550
1200	15.073	91.720	80.713	13.208	-36.771	-46.484	8.466
1300	15.166	92.930	81.607	14.720	-36.981	-47.284	7.949
1400	15.261	94.057	82.456	16.241	-37.205	-48.068	7.504
1500	15.354	95.113	83.265	17.772	-37.441	-48.835	7.115
1600	15.445	96.107	84.037	19.312	-37.690	-49.586	6.773
1667	15.503	96.742	84.535	20.349	-37.864	-50.080	6.566
1667	15.503	96.742	84.535	20.349	-38.064	-50.080	6.566
1700	15.532	97.046	84.775	20.861	-38.177	-50.317	6.469
1800	15.612	97.936	85.482	22.418	-38.531	-51.021	6.195
1811	15.620	98.031	85.557	22.590	-38.575	-51.101	6.167
1811	15.620	98.031	85.557	22.590	-41.875	-51.101	6.167
1900	15.686	98.782	86.159	23.983	-42.272	-51.542	5.929
2000	15.752	99.589	86.812	25.555	-42.715	-52.021	5.685

Phase changes: 1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.
1667 K, γ - δ transition point of Fe; ΔH° = 0.200 kcal/mol.
1811 K, melting point of Fe; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 14.328 + 0.698\times10^{-3}T - 0.690\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.328\times10^{-3}T + 0.349\times10^{-6}T^2 + 0.690\times10^{2}T^{-1} - 4.534$

$FeCl_2(g)$ - Continued

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf^\circ = -35.658 + 5.722\times10^{-3}T - 5.810\times10^{-6}T^2 + 229.200T^{-1}$

$\Delta Gf^\circ = -35.658 - 5.722\times10^{-3}T\ln T + 5.810\times10^{-6}T^2 + 114.600T^{-1} + 24.455\times10^{-3}T$

1043-1185 K: $\Delta Hf^\circ = -12.097 - 38.259\times10^{-3}T + 14.901\times10^{-6}T^2 + 0.700T^{-1}$

$\Delta Gf^\circ = -12.097 + 38.259\times10^{-3}T\ln T - 14.901\times10^{-6}T^2 + 0.350T^{-1} - 282.089\times10^{-3}T$

1185-1667 K: $\Delta Hf^\circ = -35.711 - 0.004\times10^{-3}T - 0.790\times10^{-6}T^2 + 119.700T^{-1}$

$\Delta Gf^\circ = -35.711 + 0.004\times10^{-3}T\ln T + 0.790\times10^{-6}T^2 + 59.850T^{-1} - 10.048\times10^{-3}T$

1667-1811 K: $\Delta Hf^\circ = -118.606 + 48.493\times10^{-3}T - 10.421\times10^{-6}T^2 + 47818.900T^{-1}$

$\Delta Gf^\circ = -118.606 - 48.493\times10^{-3}T\ln T + 10.421\times10^{-6}T^2 + 23909.450T^{-1} + 374.830\times10^{-3}T$

1811-2000 K: $\Delta Hf^\circ = -32.756 - 5.499\times10^{-3}T + 0.261\times10^{-6}T^2 + 0.700T^{-1}$

$\Delta Gf^\circ = -32.756 + 5.499\times10^{-3}T\ln T - 0.261\times10^{-6}T^2 + 0.350T^{-1} - 50.968\times10^{-3}T$

Source: Data from Chase (25) who estimated some molecular constants.

$(FeCl_2)_2(g)$

Dimeric Iron Dichloride (ideal gas)

[Formation: $2Fe(c,l) + 2Cl_2(g) = (FeCl_2)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	30.084	110.990	110.990	0	-103.100	-100.527	73.687
300	30.103	111.176	110.990	.056	-103.096	-100.511	73.221
400	30.795	119.944	112.182	3.105	-102.959	-99.673	54.458
500	31.140	126.857	114.451	6.203	-102.931	-98.857	43.210
600	31.337	132.553	117.006	9.328	-103.018	-98.035	35.709
700	31.467	137.394	119.581	12.469	-103.223	-97.189	30.343
800	31.567	141.602	122.077	15.620	-103.574	-96.308	26.310
900	31.656	145.326	124.457	18.782	-104.116	-95.368	23.158
1000	31.745	148.665	126.713	21.952	-105.006	-94.355	20.621
1043	31.784	150.002	127.646	23.318	-105.679	-93.884	19.672
1100	31.836	151.695	128.849	25.131	-106.285	-93.220	18.521
1185	31.918	154.068	130.575	27.840	-106.874	-92.189	17.002
1185	31.918	154.068	130.575	27.840	-107.304	-92.189	17.002
1200	31.932	154.470	130.871	28.319	-107.339	-92.001	16.755
1300	32.029	157.029	132.785	31.517	-107.585	-90.710	15.249
1400	32.128	159.407	134.603	34.725	-107.867	-89.402	13.956
1500	32.225	161.626	136.331	37.943	-108.183	-88.071	12.832
1600	32.318	163.709	137.978	41.170	-108.534	-86.718	11.845
1667	32.378	165.036	139.039	43.337	-108.788	-85.798	11.248
1667	32.378	165.036	139.039	43.337	-109.188	-85.798	11.248
1700	32.407	165.671	139.550	44.406	-109.370	-85.334	10.970
1800	32.489	167.526	141.053	47.651	-109.947	-83.905	10.187
1811	32.497	167.724	141.215	48.008	-110.020	-83.752	10.107
1811	32.497	167.724	141.215	48.008	-116.620	-83.752	10.107
1900	32.564	169.284	142.492	50.904	-117.306	-82.114	9.445
2000	32.631	170.956	143.874	54.163	-118.077	-80.245	8.769

Phase changes: 1043 K, Curie temperature of Fe; $\Delta H°$ = 0 kcal/mol.
1185 K, α - γ transition point of Fe; $\Delta H°$ = 0.215 kcal/mol.
1667 K, γ - δ transition point of Fe; $\Delta H°$ = 0.200 kcal/mol.
1811 K, melting point of Fe; $\Delta H°$ = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 31.279 + 0.646\times10^{-3}T - 1.234\times10^{5}T^{-2}$

$H°- H°_{298} = 31.279\times10^{-3}T + 0.323\times10^{-6}T^{2} + 1.234\times10^{2}T^{-1} - 9.768$

$(FeCl_2)_2(g)$ - Continued

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf^\circ = -107.716 + 14.067\times10^{-3}T - 11.995\times10^{-6}T^2 + 443.800T^{-1}$

$\Delta Gf^\circ = -107.716 - 14.067\times10^{-3}T\ln T + 11.995\times10^{-6}T^2 + 221.900T^{-1} + 98.189\times10^{-3}T$

1043-1185 K: $\Delta Hf^\circ = -60.595 - 73.895\times10^{-3}T + 29.427\times10^{-6}T^2 - 13.200T^{-1}$

$\Delta Gf^\circ = -60.595 + 73.895\times10^{-3}T\ln T - 29.427\times10^{-6}T^2 - 6.600T^{-1} - 514.900\times10^{-3}T$

1185-1667 K: $\Delta Hf^\circ = -107.822 + 2.615\times10^{-3}T - 1.955\times10^{-6}T^2 + 224.800T^{-1}$

$\Delta Gf^\circ = -107.822 - 2.615\times10^{-3}T\ln T + 1.955\times10^{-6}T^2 + 112.400T^{-1} + 29.181\times10^{-3}T$

1667-1811 K: $\Delta Hf^\circ = -273.612 + 99.609\times10^{-3}T - 21.217\times10^{-6}T^2 + 95623.200T^{-1}$

$\Delta Gf^\circ = -273.612 - 99.609\times10^{-3}T\ln T + 21.217\times10^{-6}T^2 + 47811.600T^{-1} + 798.938\times10^{-3}T$

1811-2000 K: $\Delta Hf^\circ = -101.912 - 8.375\times10^{-3}T + 0.147\times10^{-6}T^2 - 13.200T^{-1}$

$\Delta Gf^\circ = -101.912 + 8.375\times10^{-3}T\ln T - 0.147\times10^{-6}T^2 - 6.600T^{-1} - 52.658\times10^{-3}T$

Source: Data from Chase (25) who estimated most molecular constants.

$FeCl_3$(c,l)

Iron Trichloride

[Formation: $Fe(c) + 1.5Cl_2(g) = FeCl_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	23.170	35.330	35.330	0	-95.420	-80.177	58.771
300	23.207	35.473	35.330	.043	-95.410	-80.082	58.339
400	25.175	42.421	36.264	2.463	-94.862	-75.053	41.007
500	27.101	48.246	38.092	5.077	-94.209	-70.174	30.673
577	28.571	52.231	39.718	7.220	-93.631	-66.514	25.193
577	32.000	70.082	39.718	17.520	-83.331	-66.514	25.193
600	32.000	71.333	40.906	18.256	-83.071	-65.849	23.985
605	32.000	71.598	41.158	18.416	-83.014	-65.705	23.735

Phase changes: 577 K, melting point of $FeCl_3$; $\Delta H° = 10.300$ kcal/mol.
605 K, boiling point of $FeCl_3$ to equilibrium mixture of $FeCl_3(g)$ and $(FeCl_3)_2(g)$; $\Delta H° = 10.$ kcal/mol of $FeCl_3$.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-577 K: $Cp° = 17.828 + 18.708\times10^{-3}T - 0.209\times10^{5}T^{-2}$

$H°- H°_{298} = 17.828\times10^{-3}T + 9.354\times10^{-6}T^2 + 0.209\times10^{2}T^{-1} - 6.217$

577-605 K: $Cp° = 32.000$

$H°- H°_{298} = 32.000\times10^{-3}T - 0.944$

Formation equations (kcal/mol):

298.15-577 K: $\Delta Hf° = -97.627 + 4.808\times10^{-3}T + 3.151\times10^{-6}T^2 + 146.950T^{-1}$

$\Delta Gf° = -97.627 - 4.808\times10^{-3}T\ln T - 3.151\times10^{-6}T^2 + 73.475T^{-1} + 86.036\times10^{-3}T$

577-605 K: $\Delta Hf° = -92.353 + 18.981\times10^{-3}T - 6.203\times10^{-6}T^2 + 126.050T^{-1}$

$\Delta Gf° = -92.353 - 18.981\times10^{-3}T\ln T + 6.203\times10^{-6}T^2 + 63.025T^{-1} + 161.634\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (188). Low-temperature heat capacities and entropy at 298 K from Stuve (233). High-temperature data based on Todd (241).

$FeCl_3(g)$
Iron Trichloride (ideal gas)
[Formation: $Fe(c,l) + 1.5Cl_2(g) = FeCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.572	82.243	82.243	0	-60.700	-59.444	43.573
300	18.586	82.358	82.245	.034	-60.700	-59.437	43.299
400	19.117	87.787	82.979	1.923	-60.681	-59.020	32.246
500	19.379	92.084	84.386	3.849	-60.717	-58.601	25.614
600	19.526	95.632	85.974	5.795	-60.812	-58.169	21.188
700	19.616	98.649	87.575	7.752	-60.967	-57.718	18.020
800	19.675	101.272	89.126	9.717	-61.196	-57.240	15.637
900	19.716	103.592	90.606	11.687	-61.523	-56.726	13.775
1000	19.746	105.671	92.011	13.660	-62.027	-56.170	12.276
1043	19.755	106.503	92.591	14.509	-62.389	-55.912	11.716
1100	19.767	107.554	93.339	15.636	-62.728	-55.547	11.036
1185	19.781	109.026	94.413	17.316	-63.079	-54.980	10.140
1185	19.781	109.026	94.413	17.316	-63.294	-54.980	10.140
1200	19.784	109.275	94.598	17.613	-63.322	-54.875	9.994
1300	19.797	110.859	95.788	19.592	-63.516	-54.163	9.105
1400	19.807	112.326	96.917	21.573	-63.732	-53.434	8.341
1500	19.816	113.693	97.990	23.554	-63.971	-52.690	7.677
1600	19.823	114.972	99.012	25.536	-64.232	-51.929	7.093
1667	19.826	115.785	99.670	26.864	-64.419	-51.409	6.740
1667	19.826	115.785	99.670	26.864	-64.619	-51.409	6.740
1700	19.828	116.174	99.987	27.518	-64.741	-51.146	6.575
1800	19.833	117.308	100.919	29.501	-65.124	-50.338	6.112
1811	19.833	117.429	101.018	29.719	-65.171	-50.251	6.064
1811	19.833	117.429	101.018	29.719	-68.471	-50.251	6.064
1900	19.837	118.380	101.809	31.485	-68.902	-49.341	5.675
2000	19.841	119.398	102.664	33.469	-69.391	-48.300	5.278

Phase changes: 1043 K, Curie temperature of Fe; $\Delta H°$ = 0 kcal/mol.
1185 K, α - γ transition point of Fe; $\Delta H°$ = 0.215 kcal/mol.
1667 K, γ - δ transition point of Fe; $\Delta H°$ = 0.200 kcal/mol.
1811 K, melting point of Fe; $\Delta H°$ = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.809 + 0.038\times10^{-3}T - 1.110\times10^{5}T^{-2}$

$H°- H°_{298} = 19.809\times10^{-3}T + 0.019\times10^{-6}T^{2} + 1.110\times10^{2}T^{-1} - 6.280$

$FeCl_3(g)$ - Continued

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf^\circ = -62.970 + 6.790\times10^{-3}T - 6.184\times10^{-6}T^2 + 237.050T^{-1}$

$\Delta Gf^\circ = -62.970 - 6.790\times10^{-3}T\ln T + 6.184\times10^{-6}T^2 + 118.525T^{-1} + 47.331\times10^{-3}T$

1043-1185 K: $\Delta Hf^\circ = -39.409 - 37.191\times10^{-3}T + 14.527\times10^{-6}T^2 + 8.550T^{-1}$

$\Delta Gf^\circ = -39.409 + 37.191\times10^{-3}T\ln T - 14.527\times10^{-6}T^2 + 4.275T^{-1} - 259.213\times10^{-3}T$

1185-1667 K: $\Delta Hf^\circ = -63.023 + 1.063\times10^{-3}T - 1.164\times10^{-6}T^2 + 127.550T^{-1}$

$\Delta Gf^\circ = -63.023 - 1.063\times10^{-3}T\ln T + 1.164\times10^{-6}T^2 + 63.775T^{-1} + 12.828\times10^{-3}T$

1667-1811 K: $\Delta Hf^\circ = -145.918 + 49.561\times10^{-3}T - 10.795\times10^{-6}T^2 + 47826.750T^{-1}$

$\Delta Gf^\circ = -145.918 - 49.561\times10^{-3}T\ln T + 10.795\times10^{-6}T^2 + 23913.375T^{-1} + 397.706\times10^{-3}T$

1811-2000 K: $\Delta Hf^\circ = -60.068 - 4.431\times10^{-3}T - 0.113\times10^{-6}T^2 + 8.550T^{-1}$

$\Delta Gf^\circ = -60.068 + 4.431\times10^{-3}T\ln T + 0.113\times10^{-6}T^2 + 4.275T^{-1} - 28.092\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (253). Other data are those estimated by JANAF (60).

$(FeCl_3)_2(g)$

Dimeric Iron Trichloride (ideal gas)

[Formation: $2Fe(c,1) + 3Cl_2(g) = (FeCl_3)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	$C_p°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	41.508	128.350	128.350	0	-156.500	-143.214	104.978
300	41.533	128.607	128.350	.077	-156.490	-143.132	104.270
400	42.446	140.698	129.993	4.282	-156.027	-138.753	75.810
500	42.891	150.222	133.120	8.551	-155.681	-134.475	58.778
600	43.139	158.066	136.644	12.853	-155.460	-130.257	47.445
700	43.290	164.728	140.192	17.175	-155.362	-126.066	39.359
800	43.390	170.516	143.629	21.510	-155.415	-121.882	33.296
900	43.458	175.631	146.907	25.852	-155.667	-117.676	28.575
1000	43.508	180.212	150.011	30.201	-156.272	-113.430	24.790
1043	43.523	182.044	151.294	32.072	-156.825	-111.578	23.380
1100	43.544	184.361	152.948	34.554	-157.274	-109.090	21.674
1185	43.568	187.603	155.320	38.255	-157.635	-105.354	19.430
1185	43.568	187.603	155.320	38.255	-158.065	-105.354	19.430
1200	43.572	188.151	155.727	38.909	-158.061	-104.689	19.066
1300	43.594	191.639	158.356	43.268	-158.048	-100.238	16.851
1400	43.611	194.871	160.851	47.628	-158.082	-95.792	14.954
1500	43.625	197.880	163.220	51.990	-158.160	-91.340	13.308
1600	43.637	200.696	165.475	56.353	-158.283	-86.880	11.867
1667	43.643	202.486	166.928	59.277	-158.389	-83.885	10.998
1667	43.643	202.486	166.928	59.277	-158.789	-83.885	10.998
1700	43.646	203.342	167.626	60.717	-158.900	-82.402	10.593
1800	43.654	205.836	169.679	65.082	-159.268	-77.892	9.457
1811	43.655	206.102	169.900	65.562	-159.319	-77.400	9.340
1811	43.655	206.102	169.900	65.562	-165.919	-77.400	9.340
1900	43.661	208.197	171.645	69.448	-166.426	-73.033	8.401
2000	43.666	210.437	173.530	73.814	-167.005	-68.107	7.442

Phase changes: 1043 K, Curie temperature of Fe; $\Delta H°$ = 0 kcal/mol.
1185 K, α - γ transition point of Fe; $\Delta H°$ = 0.215 kcal/mol.
1667 K, γ - δ transition point of Fe; $\Delta H°$ = 0.200 kcal/mol.
1811 K, melting point of Fe; $\Delta H°$ = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p° = 43.627 + 0.058\times10^{-3}T - 1.899\times10^{5}T^{-2}$

$H°- H°_{298} = 43.627\times10^{-3}T + 0.029\times10^{-6}T^{2} + 1.899\times10^{2}T^{-1} - 13.647$

$(FeCl_3)_2(g)$ - Continued

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf^\circ = -162.126 + 17.588\times10^{-3}T - 12.377\times10^{-6}T^2 + 442.000T^{-1}$

$\Delta Gf^\circ = -162.126 - 17.588\times10^{-3}T\ln T + 12.377\times10^{-6}T^2 + 221.000T^{-1} + 157.463\times10^{-3}T$

1043-1185 K: $\Delta Hf^\circ = -115.004 - 70.374\times10^{-3}T + 29.045\times10^{-6}T^2 - 15.000T^{-1}$

$\Delta Gf^\circ = -115.004 + 70.374\times10^{-3}T\ln T - 29.045\times10^{-6}T^2 - 7.500T^{-1} - 455.626\times10^{-3}T$

1185-1667 K: $\Delta Hf^\circ = -162.232 + 6.136\times10^{-3}T - 2.337\times10^{-6}T^2 + 223.000T^{-1}$

$\Delta Gf^\circ = -162.232 - 6.136\times10^{-3}T\ln T + 2.337\times10^{-6}T^2 + 111.500T^{-1} + 88.456\times10^{-3}T$

1667-1811 K: $\Delta Hf^\circ = -328.022 + 103.130\times10^{-3}T - 21.599\times10^{-6}T^2 + 95621.400T^{-1}$

$\Delta Gf^\circ = -328.022 - 103.130\times10^{-3}T\ln T + 21.599\times10^{-6}T^2 + 47810.700T^{-1} + 858.212\times10^{-3}T$

1811-2000 K: $\Delta Hf^\circ = -156.322 - 4.854\times10^{-3}T - 0.235\times10^{-6}T^2 - 15.000T^{-1}$

$\Delta Gf^\circ = -156.322 + 4.854\times10^{-3}T\ln T + 0.235\times10^{-6}T^2 - 7.500T^{-1} + 6.617\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (253). Other data from JANAF (60) who estimated some molecular constants.

FeF(g)
Iron Monofluoride (ideal gas)
[Formation: $Fe(c,l) + 0.5F_2(g) = FeF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	7.950	57.417	57.417	0	11.400	3.447	-2.526
300	7.959	57.467	57.417	.015	11.397	3.397	-2.475
400	8.306	59.808	57.736	.829	11.201	.759	-.415
500	8.518	61.686	58.342	1.672	10.959	-1.824	.797
600	8.652	63.252	59.034	2.531	10.667	-4.354	1.586
700	8.743	64.593	59.734	3.401	10.318	-6.830	2.132
800	8.807	65.765	60.417	4.278	9.898	-9.253	2.528
900	8.854	66.805	61.071	5.161	9.384	-11.617	2.821
1000	8.891	67.740	61.691	6.049	8.696	-13.916	3.041
1043	8.904	68.115	61.948	6.432	8.254	-14.880	3.118
1100	8.921	68.589	62.281	6.939	7.811	-16.132	3.205
1185	8.942	69.253	62.757	7.699	7.308	-17.962	3.313
1185	8.942	69.253	62.757	7.699	7.093	-17.962	3.313
1200	8.946	69.366	62.838	7.833	7.038	-18.280	3.329
1300	8.967	70.083	63.369	8.728	6.666	-20.374	3.425
1400	8.985	70.748	63.872	9.626	6.273	-22.440	3.503
1500	9.002	71.369	64.352	10.525	5.859	-24.477	3.566
1600	9.017	71.950	64.809	11.426	5.427	-26.484	3.617
1667	9.026	72.320	65.103	12.031	5.126	-27.814	3.646
1667	9.026	72.320	65.103	12.031	4.926	-27.814	3.646
1700	9.030	72.497	65.245	12.329	4.748	-28.460	3.659
1800	9.043	73.014	65.663	13.232	4.195	-30.399	3.691
1811	9.044	73.069	65.708	13.331	4.130	-30.613	3.694
1811	9.044	73.069	65.708	13.331	.830	-30.613	3.694
1900	9.055	73.503	66.062	14.137	.250	-32.143	3.697
2000	9.067	73.968	66.447	15.043	-.403	-33.833	3.697

*All data estimated.

Phase changes: 1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.
1667 K, γ - δ transition point of Fe; ΔH° = 0.200 kcal/mol.
1811 K, melting point of Fe; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.725 + 0.214\times10^{-3}T - 0.745\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.725\times10^{-3}T + 0.107\times10^{-6}T^2 + 0.745\times10^{2}T^{-1} - 2.861$

FeF(g) - Continued

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf^\circ = 9.691 + 4.692\times10^{-3}T - 6.051\times10^{-6}T^2 + 252.750T^{-1}$

$\Delta Gf^\circ = 9.691 - 4.692\times10^{-3}T\ln T + 6.051\times10^{-6}T^2 + 126.375T^{-1} + 2.563\times10^{-3}T$

1043-1185 K: $\Delta Hf^\circ = 33.252 - 39.289\times10^{-3}T + 14.660\times10^{-6}T^2 + 24.250T^{-1}$

$\Delta Gf^\circ = 33.252 + 39.289\times10^{-3}T\ln T - 14.660\times10^{-6}T^2 + 12.125T^{-1} - 303.981\times10^{-3}T$

1185-1667 K: $\Delta Hf^\circ = 9.638 - 1.034\times10^{-3}T - 1.031\times10^{-6}T^2 + 143.250T^{-1}$

$\Delta Gf^\circ = 9.638 + 1.034\times10^{-3}T\ln T + 1.031\times10^{-6}T^2 + 71.625T^{-1} - 31.941\times10^{-3}T$

1667-1811 K: $\Delta Hf^\circ = -73.257 + 47.463\times10^{-3}T - 10.662\times10^{-6}T^2 + 47842.450T^{-1}$

$\Delta Gf^\circ = -73.257 - 47.463\times10^{-3}T\ln T + 10.662\times10^{-6}T^2 + 23921.225T^{-1} + 352.938\times10^{-3}T$

1811-2000 K: $\Delta Hf^\circ = 12.593 - 6.529\times10^{-3}T + 0.020\times10^{-6}T^2 + 24.250T^{-1}$

$\Delta Gf^\circ = 12.593 + 6.529\times10^{-3}T\ln T - 0.020\times10^{-6}T^2 + 12.125T^{-1} - 72.860\times10^{-3}T$

Source: Data estimated by JANAF (60).

FeF_2(c,l)
Iron Difluoride
[Formation: Fe(c) + F_2(g) = FeF_2(c,l)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	16.280	20.790	20.790	0	-168.700	-158.511	116.190
300	16.300	20.891	20.791	.030	-168.695	-158.448	115.428
400	17.200	25.708	21.441	1.707	-168.413	-155.075	84.728
500	17.900	29.624	22.698	3.463	-168.143	-151.772	66.339
600	18.440	32.938	24.136	5.281	-167.892	-148.522	54.098
700	18.850	35.812	25.603	7.146	-167.670	-145.311	45.368
800	19.180	38.351	27.041	9.048	-167.495	-142.131	38.828
900	19.440	40.626	28.426	10.980	-167.396	-138.966	33.745
1000	19.630	42.684	29.750	12.934	-167.458	-135.807	29.680
1043	19.690	43.512	30.300	13.779	-167.627	-134.443	28.171
1100	19.769	44.562	31.013	14.904	-167.706	-132.626	26.350
1185	19.863	46.037	32.038	16.589	-167.662	-129.917	23.960
1185	19.863	46.037	32.038	16.589	-167.877	-129.917	23.960
1200	19.880	46.287	32.215	16.887	-167.835	-129.437	23.573
1213	19.889	46.501	32.367	17.145	-167.799	-129.022	23.246
1213	23.500	55.487	32.367	28.045	-156.899	-129.022	23.246
1300	23.500	57.115	33.969	30.090	-156.347	-127.040	21.357
1400	23.500	58.856	35.685	32.440	-155.738	-124.809	19.483
1500	23.500	60.478	37.285	34.790	-155.152	-122.622	17.866
1600	23.500	61.994	38.782	37.140	-154.589	-120.469	16.455
1667	23.500	62.958	39.734	38.715	-154.224	-119.048	15.607
1667	23.500	62.958	39.734	38.715	-154.424	-119.048	15.607
1700	23.500	63.419	40.190	39.490	-154.274	-118.350	15.215
1800	23.500	64.762	41.518	41.840	-153.836	-116.248	14.114

*Data above 298 K estimated except temperature of fusion.

Phase changes: 1043 K, Curie temperature of Fe; $\Delta H°$ = 0 kcal/mol.
1185 K, α - γ transition point of Fe; $\Delta H°$ = 0.215 kcal/mol.
1213 K, melting point of FeF_2; $\Delta H°$ = 10.900 kcal/mol.
1667 K, γ - δ transition point of Fe; $\Delta H°$ = 0.200 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1213 K: $Cp° = 17.466 + 2.296\times10^{-3}T - 1.662\times10^{5}T^{-2}$

$H°- H°_{298} = 17.466\times10^{-3}T + 1.148\times10^{-6}T^{2} + 1.662\times10^{2}T^{-1} - 5.867$

1213-1800 K: $Cp° = 23.500$

$H°- H°_{298} = 23.500\times10^{-3}T - 0.460$

FeF_2(c,1) - Continued

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf^\circ = -171.970 + 9.179\times10^{-3}T - 5.097\times10^{-6}T^2 + 294.200T^{-1}$

$\Delta Gf^\circ = -171.970 - 9.179\times10^{-3}T\ln T + 5.097\times10^{-6}T^2 + 147.100T^{-1} + 94.266\times10^{-3}T$

1043-1185 K: $\Delta Hf^\circ = -148.410 - 34.802\times10^{-3}T + 15.614\times10^{-6}T^2 + 65.700T^{-1}$

$\Delta Gf^\circ = -148.410 + 34.802\times10^{-3}T\ln T - 15.614\times10^{-6}T^2 + 32.850T^{-1} - 212.279\times10^{-3}T$

1185-1213 K: $\Delta Hf^\circ = -172.023 + 3.453\times10^{-3}T - 0.077\times10^{-6}T^2 + 184.700T^{-1}$

$\Delta Gf^\circ = -172.023 - 3.453\times10^{-3}T\ln T + 0.077\times10^{-6}T^2 + 92.350T^{-1} + 59.762\times10^{-3}T$

1213-1667 K: $\Delta Hf^\circ = -166.617 + 9.487\times10^{-3}T - 1.225\times10^{-6}T^2 + 18.500T^{-1}$

$\Delta Gf^\circ = -166.617 - 9.487\times10^{-3}T\ln T + 1.225\times10^{-6}T^2 + 9.250T^{-1} + 96.815\times10^{-3}T$

1667-1800 K: $\Delta Hf^\circ = -249.511 + 57.984\times10^{-3}T - 10.856\times10^{-6}T^2 + 47717.700T^{-1}$

$\Delta Gf^\circ = -249.511 - 57.984\times10^{-3}T\ln T + 10.856\times10^{-6}T^2 + 23858.850T^{-1} + 481.693\times10^{-3}T$

Sources: Temperature of fusion from Petrov (193). Other data from JANAF (60) who estimated data above 298 K. Enthalpy of fusion calculated from JANAF's estimated entropy of fusion.

$FeF_2(g)$
Iron Difluoride (ideal gas)
[Formation: $Fe(c,l) + F_2(g) = FeF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	13.324	63.361	63.361	0	-93.100	-95.604	70.079
300	13.355	63.444	63.361	.025	-93.100	-95.619	69.658
400	14.673	67.482	63.902	1.432	-93.088	-96.459	52.702
500	15.365	70.841	64.965	2.938	-93.068	-97.305	42.532
600	15.647	73.672	66.187	4.491	-93.082	-98.153	35.752
700	15.723	76.091	67.432	6.061	-93.155	-98.992	30.906
800	15.714	78.191	68.650	7.633	-93.310	-99.818	27.269
900	15.679	80.040	69.814	9.203	-93.573	-100.616	24.432
1000	15.644	81.690	70.921	10.769	-94.023	-101.378	22.156
1043	15.632	82.348	71.379	11.441	-94.365	-101.688	21.307
1100	15.617	83.179	71.968	12.332	-94.678	-102.077	20.280
1185	15.603	84.341	72.814	13.659	-94.992	-102.637	18.929
1185	15.603	84.341	72.814	13.659	-95.207	-102.637	18.929
1200	15.600	84.537	72.960	13.893	-95.229	-102.731	18.710
1300	15.591	85.786	73.900	15.452	-95.385	-103.350	17.375
1400	15.588	86.941	74.790	17.011	-95.567	-103.957	16.228
1500	15.590	88.016	75.636	18.570	-95.772	-104.549	15.233
1600	15.594	89.023	76.442	20.129	-96.000	-105.126	14.359
1667	15.597	89.662	76.960	21.174	-96.165	-105.504	13.8321
1667	15.597	89.662	76.960	21.174	-96.365	-105.504	13.832
1700	15.599	89.968	77.210	21.689	-96.475	-105.684	13.586
1800	15.604	90.860	77.944	23.249	-96.827	-106.216	12.896
1811	15.605	90.955	78.023	23.421	-96.871	-106.276	12.825
1811	15.605	90.955	78.023	23.421	-100.171	-106.276	12.825
1900	15.609	91.704	78.646	24.810	-100.573	-106.566	12.258
2000	15.612	92.504	79.318	26.371	-101.029	-106.869	11.678

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1043 K, Curie temperature of Fe; $\Delta H°$ = 0 kcal/mol.
1185 K, α - γ transition point of Fe; $\Delta H°$ = 0.215 kcal/mol.
1667 K, γ - δ transition point of Fe; $\Delta H°$ = 0.200 kcal/mol.
1811 K, melting point of Fe; $\Delta H°$ = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 16.860 - 0.794\times10^{-3}T - 2.933\times10^{5}T^{-2}$

$H°- H°_{298} = 16.860\times10^{-3}T - 0.397\times10^{-6}T^{2} + 2.933\times10^{2}T^{-1} - 5.975$

$FeF_2(g)$ - Continued

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf^\circ = -96.479 + 8.573\times10^{-3}T - 6.642\times10^{-6}T^2 + 421.300T^{-1}$

$\Delta Gf^\circ = -96.479 - 8.573\times10^{-3}T\ln T + 6.642\times10^{-6}T^2 + 210.650T^{-1} + 47.430\times10^{-3}T$

1043-1185 K: $\Delta Hf^\circ = -72.918 - 35.408\times10^{-3}T + 14.069\times10^{-6}T^2 + 192.800T^{-1}$

$\Delta Gf^\circ = -72.918 + 35.408\times10^{-3}T\ln T - 14.069\times10^{-6}T^2 + 96.400T^{-1} - 259.115\times10^{-3}T$

1185-1667 K: $\Delta Hf^\circ = -96.532 + 2.847\times10^{-3}T - 1.622\times10^{-6}T^2 + 311.800T^{-1}$

$\Delta Gf^\circ = -96.532 - 2.847\times10^{-3}T\ln T + 1.622\times10^{-6}T^2 + 155.900T^{-1} + 12.926\times10^{-3}T$

1667-1811 K: $\Delta Hf^\circ = -179.427 + 51.344\times10^{-3}T - 11.253\times10^{-6}T^2 + 48011.000T^{-1}$

$\Delta Gf^\circ = -179.427 - 51.344\times10^{-3}T\ln T + 11.253\times10^{-6}T^2 + 24005.500T^{-1} + 397.804\times10^{-3}T$

1811-2000 K: $\Delta Hf^\circ = -93.577 - 2.648\times10^{-3}T - 0.571\times10^{-6}T^2 + 192.800T^{-1}$

$\Delta Gf^\circ = -93.577 + 2.648\times10^{-3}T\ln T + 0.571\times10^{-6}T^2 + 96.400T^{-1} - 27.994\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$FeF_3(c)$

Iron Trifluoride

[Formation: $Fe(c) + 1.5F_2(g) = FeF_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	21.750	23.500	23.500	0	-248.400	-231.798	169.910
300	21.900	23.635	23.502	.040	-248.392	-231.695	168.788
400	23.033	30.477	24.420	2.423	-247.788	-226.218	123.598
500*	22.865	35.584	26.162	4.711	-247.388	-220.874	96.543
600	23.140	39.778	28.093	7.011	-247.070	-215.603	78.532
700	23.440	43.367	30.024	9.340	-246.809	-210.379	65.682
800	23.740	46.517	31.893	11.699	-246.607	-205.191	56.055
900	24.040	49.330	33.677	14.088	-246.487	-200.020	48.571
1000	24.340	51.879	35.372	16.507	-246.524	-194.860	42.586
1043	24.469	52.906	36.074	17.556	-246.679	-192.636	40.364
1100	24.640	54.212	36.979	18.956	-246.736	-189.678	37.685
1185	24.895	56.056	38.282	21.061	-246.650	-185.272	34.169
1185	24.895	56.056	38.282	21.061	-246.865	-185.272	34.169
1200	24.940	56.369	38.507	21.435	-246.814	-184.494	33.601

*Data above 450 K estimated.

Phase changes: 1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1185 K, $\alpha - \gamma$ transition point of Fe; ΔH° = 0.215 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp^\circ = 25.185 - 0.836\times10^{-3}T - 2.832\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.185\times10^{-3}T - 0.418\times10^{-6}T^2 + 2.832\times10^{2}T^{-1} - 8.422$

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf^\circ = -252.780 + 12.644\times10^{-3}T - 6.750\times10^{-6}T^2 + 360.950T^{-1}$

$\Delta Gf^\circ = -252.780 - 12.644\times10^{-3}T\ln T + 6.750\times10^{-6}T^2 + 180.475T^{-1} + 138.374\times10^{-3}T$

1043-1185 K: $\Delta Hf^\circ = -229.220 - 31.337\times10^{-3}T + 13.961\times10^{-6}T^2 + 132.450T^{-1}$

$\Delta Gf^\circ = -229.220 + 31.337\times10^{-3}T\ln T - 13.961\times10^{-6}T^2 + 66.225T^{-1} - 168.170\times10^{-3}T$

1185-1200 K: $\Delta Hf^\circ = -252.833 + 6.918\times10^{-3}T - 1.730\times10^{-6}T^2 + 251.450T^{-1}$

$\Delta Gf^\circ = -252.833 - 6.918\times10^{-3}T\ln T + 1.730\times10^{-6}T^2 + 125.725T^{-1} + 103.870\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Schaefer (204). Other data from JANAF (60) who estimated data above 450 K. Their data includes a heat capacity peak at 367 K.

$FeF_3(g)$

Iron Trifluoride (ideal gas)

[Formation: $Fe(c,l) + 1.5F_2(g) = FeF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	15.666	72.690	72.690	0	-196.200	-194.264	142.397
300	15.697	72.787	72.690	.029	-196.203	-194.252	141.511
400	17.027	77.500	73.325	1.670	-196.341	-193.580	105.766
500	17.858	81.396	74.560	3.418	-196.481	-192.873	84.304
600	18.389	84.702	75.982	5.232	-196.650	-192.137	69.985
700	18.742	87.565	77.436	7.090	-196.859	-191.368	59.747
800	18.986	90.084	78.863	8.977	-197.129	-190.567	52.060
900	19.160	92.331	80.237	10.885	-197.490	-189.724	46.071
1000	19.288	94.357	81.550	12.807	-198.024	-188.838	41.270
1043	19.330	95.170	82.095	13.637	-198.398	-188.436	39.484
1100	19.385	96.200	82.799	14.741	-198.751	-187.880	37.328
1185	19.449	97.645	83.812	16.392	-199.119	-187.026	34.493
1185	19.449	97.645	83.812	16.392	-199.334	-187.026	34.493
1200	19.460	97.890	83.987	16.684	-199.365	-186.870	34.033
1300	19.519	99.450	85.117	18.633	-199.579	-185.819	31.239
1400	19.566	100.898	86.193	20.587	-199.816	-184.753	28.841
1500	19.605	102.250	87.219	22.546	-200.072	-183.669	26.760
1600	19.637	103.516	88.199	24.508	-200.351	-182.565	24.937
1667	19.654	104.322	88.830	25.824	-200.548	-181.815	23.836
1667	19.654	104.322	88.830	25.824	-200.748	-181.815	23.836
1700	19.663	104.707	89.135	26.473	-200.875	-181.439	23.325
1800	19.685	105.832	90.032	28.440	-201.275	-180.286	21.889
1811	19.687	105.952	90.128	28.657	-201.325	-180.161	21.741
1811	19.687	105.952	90.128	28.657	-204.625	-180.161	21.741
1900	19.704	106.897	90.892	30.410	-205.069	-178.946	20.583
2000	19.720	107.908	91.717	32.381	-205.574	-177.559	19.403

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.
1667 K, γ - δ transition point of Fe; ΔH° = 0.200 kcal/mol.
1811 K, melting point of Fe; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 18.784 + 0.670\times10^{-3}T - 2.949\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 18.784\times10^{-3}T + 0.335\times10^{-6}T^2 + 2.949\times10^{2}T^{-1} - 6.619$

$FeF_3(g)$ - Continued

Formation equations (kcal/mol):

298.15-1043 K: $\Delta Hf^\circ = -198.778 + 6.243\times10^{-3}T - 5.997\times10^{-6}T^2 + 372.650T^{-1}$

$\Delta Gf^\circ = -198.778 - 6.243\times10^{-3}T\ln T + 5.997\times10^{-6}T^2 + 186.325T^{-1} + 46.828\times10^{-3}T$

1043-1185 K: $\Delta Hf^\circ = -175.217 - 37.738\times10^{-3}T + 14.714\times10^{-6}T^2 + 144.150T^{-1}$

$\Delta Gf^\circ = -175.217 + 37.738\times10^{-3}T\ln T - 14.714\times10^{-6}T^2 + 72.075T^{-1} - 259.717\times10^{-3}T$

1185-1667 K: $\Delta Hf^\circ = -198.831 + 0.517\times10^{-3}T - 0.977\times10^{-6}T^2 + 263.150T^{-1}$

$\Delta Gf^\circ = -198.831 - 0.517\times10^{-3}T\ln T + 0.977\times10^{-6}T^2 + 131.575T^{-1} + 12.324\times10^{-3}T$

1667-1811 K: $\Delta Hf^\circ = -281.726 + 49.014\times10^{-3}T - 10.608\times10^{-6}T^2 + 47962.350T^{-1}$

$\Delta Gf^\circ = -281.726 - 49.014\times10^{-3}T\ln T + 10.608\times10^{-6}T^2 + 23981.175T^{-1} + 397.202\times10^{-3}T$

1811-2000 K: $\Delta Hf^\circ = -195.876 - 4.978\times10^{-3}T + 0.074\times10^{-6}T^2 + 144.150T^{-1}$

$\Delta Gf^\circ = -195.876 + 4.978\times10^{-3}T\ln T - 0.074\times10^{-6}T^2 + 72.075T^{-1} - 28.596\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

FeI_2(c,1)
Iron Diiodide
[Formation: Fe(c) + I_2(c,1,g) = FeI_2(c,1)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	20.000	40.000	40.000	0	-25.000	-26.706	19.576
300	20.000	40.124	40.001	.037	-24.998	-26.716	19.463
386.8	20.052	45.213	40.623	1.775	-25.008	-27.217	15.378
386.8	20.052	45.213	40.623	1.775	-28.717	-27.217	15.378
400	20.060	45.886	40.786	2.040	-28.793	-27.165	14.842
458.4	20.095	48.621	41.613	3.213	-29.137	-26.901	12.825
458.4	20.095	48.621	41.613	3.213	-39.158	-26.901	12.825
500	20.120	50.368	42.270	4.049	-38.984	-25.795	11.275
600	20.178	54.042	43.935	6.064	-38.603	-23.194	8.448
650	20.207	55.659	44.775	7.075	-38.430	-21.916	7.369
650	20.920	55.967	44.775	7.275	-38.230	-21.916	7.369
700	22.800	57.588	45.634	8.368	-37.993	-20.671	6.454
800*	26.500	60.874	47.332	10.834	-37.293	-18.239	4.983
860	28.709	62.879	48.344	12.500	-36.730	-16.829	4.277
860	27.000	75.321	48.344	23.200	-26.030	-16.829	4.277
900	27.000	76.549	49.571	24.280	-25.713	-16.409	3.985
1000	27.000	79.394	52.414	26.980	-25.054	-15.413	3.368
1043	27.000	80.531	53.550	28.141	-24.917	-15.002	3.143
1100	27.000	81.967	54.985	29.680	-24.593	-14.468	2.874
1185	27.000	83.977	56.994	31.975	-23.955	-13.709	2.528
1185	27.000	83.977	56.994	31.975	-24.170	-13.709	2.528
1200	27.000	84.317	57.334	32.380	-24.023	-13.579	2.473
1300	27.000	86.478	59.493	35.080	-23.052	-12.747	2.143
1336	27.000	87.216	60.231	36.052	-22.708	-12.467	2.039

*Heat capacities 298-343 K and above 773 K estimated. Enthalpy of fusion estimated.

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
650 K, α - β transition point of FeI_2; $\Delta H°$ = 0.200 kcal/mol.
860 K, melting point of FeI_2; $\Delta H°$ = 10.700 kcal/mol.
1043 K, Curie temperature of Fe; $\Delta H°$ = 0 kcal/mol.
1185 K, α - γ transition point of Fe; $\Delta H°$ = 0.215 kcal/mol.
1336 K boiling point of FeI_2 to equilibrium mixture of FeI_2(g) and $(FeI_2)_2$(g); $\Delta H°$ = 25 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-650 K: $Cp° = 19.658 + 0.868\times10^{-3}T + 0.074\times10^{5}T^{-2}$
$H°- H°_{298} = 19.658\times10^{-3}T + 0.434\times10^{-6}T^2 - 0.074\times10^{2}T^{-1} - 5.875$

650-860 K: $Cp° = -4.183 + 38.262\times10^{-3}T + 0.980\times10^{5}T^{-2}$
$H°- H°_{298} = -4.183\times10^{-3}T + 19.131\times10^{-6}T^2 - 0.980\times10^{2}T^{-1} + 2.062$

860-1336 K: $Cp° = 27.000$
$H°- H°_{298} = 27.000\times10^{-3}T - 0.020$

FeI_2(c,l) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -27.195 + 7.002\times10^{-3}T - 7.129\times10^{-6}T^2 + 221.100T^{-1}$

$\Delta Gf^\circ = -27.195 - 7.002\times10^{-3}T\ln T + 7.129\times10^{-6}T^2 + 110.550T^{-1} + 38.167\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -28.651 + 0.598\times10^{-3}T - 5.637\times10^{-6}T^2 + 221.100T^{-1}$

$\Delta Gf^\circ = -28.651 - 0.598\times10^{-3}T\ln T + 5.637\times10^{-6}T^2 + 110.550T^{-1} + 4.352\times10^{-3}T$

458.4-650 K: $\Delta Hf^\circ = -43.364 + 10.938\times10^{-3}T - 5.705\times10^{-6}T^2 + 205.800T^{-1}$

$\Delta Gf^\circ = -43.364 - 10.938\times10^{-3}T\ln T + 5.705\times10^{-6}T^2 + 102.900T^{-1} + 99.815\times10^{-3}T$

650-860 K: $\Delta Hf^\circ = -35.427 - 12.903\times10^{-3}T + 12.992\times10^{-6}T^2 + 115.200T^{-1}$

$\Delta Gf^\circ = -35.427 + 12.903\times10^{-3}T\ln T - 12.992\times10^{-6}T^2 + 57.600T^{-1} - 54.553\times10^{-3}T$

860-1043 K: $\Delta Hf^\circ = -37.509 + 18.280\times10^{-3}T - 6.139\times10^{-6}T^2 + 213.200T^{-1}$

$\Delta Gf^\circ = -37.509 - 18.280\times10^{-3}T\ln T + 6.139\times10^{-6}T^2 + 106.600T^{-1} + 142.051\times10^{-3}T$

1043-1185 K: $\Delta Hf^\circ = -13.949 - 25.701\times10^{-3}T + 14.572\times10^{-6}T^2 - 15.300T^{-1}$

$\Delta Gf^\circ = -13.949 + 25.701\times10^{-3}T\ln T - 14.572\times10^{-6}T^2 - 7.650T^{-1} - 164.494\times10^{-3}T$

1185-1336 K: $\Delta Hf^\circ = -37.562 + 12.554\times10^{-3}T - 1.119\times10^{-6}T^2 + 103.700T^{-1}$

$\Delta Gf^\circ = -37.562 - 12.554\times10^{-3}T\ln T + 1.119\times10^{-6}T^2 + 51.850T^{-1} + 107.547\times10^{-3}T$

Source: Data from JANAF (60) who estimated heat capacities 298-343 K and above 773 K. They also estimated enthalpy of fusion.

$FeI_2(g)$

Iron Diiodide (ideal gas)

[Formation: $Fe(c,l) + I_2(c,l,g) = FeI_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	14.545	83.530	83.530	0	21.000	6.316	-4.629
300	14.549	83.620	83.530	.027	20.992	6.225	-4.535
386.8	14.678	87.335	83.984	1.296	20.513	2.011	-1.136
386.8	14.678	87.335	83.984	1.296	16.804	2.011	-1.136
400	14.698	87.828	84.103	1.490	16.657	1.508	-.824
458.4	14.741	89.835	84.708	2.350	16.001	-.656	.313
458.4	14.741	89.835	84.708	2.350	5.980	-.656	.313
500	14.772	91.117	85.189	2.964	5.931	-1.254	.548
600	14.819	93.815	86.408	4.444	5.777	-2.678	.976
700	14.861	96.102	87.633	5.928	5.567	-4.071	1.271
800	14.911	98.090	88.820	7.416	5.289	-5.430	1.483
900	14.972	99.849	89.949	8.910	4.917	-6.749	1.639
1000	15.046	101.430	91.019	10.411	4.377	-8.018	1.752
1043	15.083	102.064	91.461	11.059	4.001	-8.544	1.790
1100	15.131	102.868	92.032	11.920	3.647	-9.219	1.832
1185	15.208	103.998	92.850	13.210	3.280	-10.199	1.881
1185	15.208	103.998	92.850	13.210	3.065	-10.199	1.881
1200	15.222	104.189	92.991	13.438	3.035	-10.368	1.888
1300	15.317	105.411	93.900	14.964	2.832	-11.476	1.929
1400	15.411	106.550	94.764	16.501	2.616	-12.568	1.962
1500	15.502	107.616	95.585	18.047	2.388	-13.645	1.988
1600	15.588	108.619	96.368	19.601	2.147	-14.704	2.008
1667	15.641	109.260	96.874	20.647	1.978	-15.409	2.020
1667	15.641	109.260	96.874	20.647	1.778	-15.409	2.020
1700	15.667	109.567	97.118	21.164	1.667	-15.748	2.024
1800	15.738	110.464	97.834	22.734	1.320	-16.761	2.035
1811	15.745	110.560	97.911	22.907	1.277	-16.875	2.036
1811	15.745	110.560	97.911	22.907	-2.023	-16.875	2.036
1900	15.801	111.317	98.522	24.311	-2.416	-17.595	2.024
2000	15.856	112.129	99.182	25.894	-2.853	-18.383	2.009

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
1043 K, Curie temperature of Fe; $\Delta H°$ = 0 kcal/mol.
1185 K, α - γ transition point of Fe; $\Delta H°$ = 0.215 kcal/mol.
1667 K, γ - δ transition point of Fe; $\Delta H°$ = 0.200 kcal/mol.
1811 K, melting point of Fe; $\Delta H°$ = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 14.397 + 0.716\times10^{-3}T - 0.058\times10^{5}T^{-2}$

$H°- H°_{298} = 14.397\times10^{-3}T + 0.358\times10^{-6}T^{2} + 0.058\times10^{2}T^{-1} - 4.344$

$FeI_2(g)$ - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = 20.336 + 1.741\times10^{-3}T - 7.205\times10^{-6}T^2 + 234.300T^{-1}$

$\Delta Gf^\circ = 20.336 - 1.741\times10^{-3}T\ln T + 7.205\times10^{-6}T^2 + 117.150T^{-1} - 40.570\times10^{-2}T$

386.8-458.4 K: $\Delta Hf^\circ = 18.880 - 4.663\times10^{-3}T - 5.713\times10^{-6}T^2 + 234.300T^{-1}$

$\Delta Gf^\circ = 18.880 + 4.663\times10^{-3}T\ln T + 5.713\times10^{-6}T^2 + 117.150T^{-1} - 74.385\times10^{-3}T$

458.4-1043 K: $\Delta Hf^\circ = 4.167 + 5.677\times10^{-3}T - 5.781\times10^{-6}T^2 + 219.000T^{-1}$

$\Delta Gf^\circ = 4.167 - 5.677\times10^{-3}T\ln T + 5.781\times10^{-6}T^2 + 109.500T^{-1} + 21.078\times10^{-3}T$

1043-1185 K: $\Delta Hf^\circ = 27.728 - 38.304\times10^{-3}T + 14.930\times10^{-6}T^2 - 9.500T^{-1}$

$\Delta Gf^\circ = 27.728 + 38.304\times10^{-3}T\ln T - 14.930\times10^{-6}T^2 - 4.750T^{-1} - 285.467\times10^{-3}T$

1185-1667 K: $\Delta Hf^\circ = 4.114 - 0.049\times10^{-3}T - 0.761\times10^{-6}T^2 + 109.500T^{-1}$

$\Delta Gf^\circ = 4.114 + 0.049\times10^{-3}T\ln T + 0.761\times10^{-6}T^2 + 54.750T^{-1} - 13.426\times10^{-3}T$

1667-1811 K: $\Delta Hf^\circ = -78.781 + 48.448\times10^{-3}T - 10.392\times10^{-6}T^2 + 47808.700T^{-1}$

$\Delta Gf^\circ = -78.781 - 48.448\times10^{-3}T\ln T + 10.392\times10^{-6}T^2 + 23904.350T^{-1} + 371.452\times10^{-3}T$

1811-2000 K: $\Delta Hf^\circ = 7.069 - 5.544\times10^{-3}T + 0.290\times10^{-6}T^2 - 9.500T^{-1}$

$\Delta Gf^\circ = 7.069 + 5.544\times10^{-3}T\ln T - 0.290\times10^{-6}T^2 - 4.750T^{-1} - 54.346\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$(FeI_2)_2(g)$

Dimeric Iron Diiodide (ideal gas)

[Formation: $2Fe(c,l) + 2I_2(c,l,g) = (FeI_2)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	31.377	129.865	129.865	0	2.000	-16.279	11.933
300	31.382	130.059	129.866	.058	1.988	-16.392	11.941
386.8	31.537	138.056	130.844	2.790	1.223	-21.619	12.215
386.8	31.537	138.056	130.844	2.790	-6.195	-21.619	12.215
400	31.561	139.115	131.100	3.206	-6.460	-22.141	12.097
458.4	31.611	143.421	132.401	5.051	-7.648	-24.344	11.606
458.4	31.611	143.421	132.401	5.051	-27.690	-24.344	11.606
500	31.646	146.168	133.434	6.367	-27.699	-24.037	10.506
600	31.699	151.942	136.050	9.535	-27.799	-23.297	8.486
700	31.744	156.832	138.679	12.707	-28.015	-22.530	7.034
800	31.797	161.074	141.219	15.884	-28.370	-21.724	5.935
900	31.861	164.823	143.639	19.066	-28.920	-20.864	5.066
1000	31.939	168.184	145.928	22.256	-29.812	-19.926	4.355
1043	31.978	169.529	146.873	23.630	-30.485	-19.488	4.083
1100	32.029	171.232	148.091	25.455	-31.091	-18.868	3.749
1185	32.114	173.619	149.837	28.181	-31.678	-17.900	3.301
1185	32.114	173.619	149.837	28.181	-32.108	-17.900	3.301
1200	32.129	174.023	150.137	28.663	-32.143	-17.723	3.228
1300	32.235	176.599	152.075	31.881	-32.383	-16.509	2.775
1400	32.343	178.992	153.913	35.110	-32.660	-15.278	2.385
1500	32.450	181.227	155.661	38.349	-32.969	-14.029	2.044
1600	32.554	183.325	157.325	41.600	-33.308	-12.750	1.741
1667	32.620	184.661	158.397	43.783	-33.556	-11.886	1.558
1667	32.620	184.661	158.397	43.783	-33.956	-11.886	1.558
1700	32.653	185.301	158.913	44.860	-34.134	-11.448	1.472
1800	32.744	187.170	160.431	48.130	-34.698	-10.096	1.226
1811	32.753	187.370	160.594	48.490	-34.770	-9.952	1.201
1811	32.753	187.370	160.594	48.490	-41.370	-9.952	1.201
1900	32.826	188.943	161.886	51.408	-42.046	-8.391	.965
2000	32.900	190.628	163.281	54.695	-42.799	-6.599	.721

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.
1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.
1667 K, γ - δ transition point of Fe; ΔH° = 0.200 kcal/mol.
1811 K, melting point of Fe; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 31.244 + 0.782\times10^{-3}T - 0.089\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 31.244\times10^{-3}T + 0.391\times10^{-6}T^2 + 0.089\times10^{2}T^{-1} - 9.380$

$(FeI_2)_2(g)$ - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -0.021 + 5.932\times10^{-3}T - 14.735\times10^{-6}T^2 + 465.900T^{-1}$

$\Delta Gf^\circ = -0.021 - 5.932\times10^{-3}T\ln T + 14.735\times10^{-6}T^2 + 232.950T^{-1} - 27.745\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -2.932 - 6.876\times10^{-3}T - 11.751\times10^{-6}T^2 + 465.900T^{-1}$

$\Delta Gf^\circ = -2.932 + 6.876\times10^{-3}T\ln T + 11.751\times10^{-6}T^2 + 232.950T^{-1} - 95.375\times10^{-3}T$

458.4-1043 K: $\Delta Hf^\circ = -32.358 + 13.804\times10^{-3}T - 11.887\times10^{-6}T^2 + 435.300T^{-1}$

$\Delta Gf^\circ = -32.358 - 13.804\times10^{-3}T\ln T + 11.887\times10^{-6}T^2 + 217.650T^{-1} + 95.550\times10^{-3}T$

1043-1185 K: $\Delta Hf^\circ = 14.764 - 74.158\times10^{-3}T + 29.535\times10^{-6}T^2 - 21.700T^{-1}$

$\Delta Gf^\circ = 14.764 + 74.158\times10^{-3}T\ln T - 29.535\times10^{-6}T^2 - 10.850T^{-1} - 517.539\times10^{-3}T$

1185-1667 K: $\Delta Hf^\circ = -32.464 + 2.352\times10^{-3}T - 1.847\times10^{-6}T^2 + 216.300T^{-1}$

$\Delta Gf^\circ = -32.464 - 2.352\times10^{-3}T\ln T + 1.847\times10^{-6}T^2 + 108.150T^{-1} + 26.543\times10^{-3}T$

1667-1811 K: $\Delta Hf^\circ = -198.254 + 99.346\times10^{-3}T - 21.109\times10^{-6}T^2 + 95614.700T^{-1}$

$\Delta Gf^\circ = -198.254 - 99.346\times10^{-3}T\ln T + 21.109\times10^{-6}T^2 + 47807.350T^{-1} + 796.300\times10^{-3}T$

1811-2000 K: $\Delta Hf^\circ = -26.554 - 8.638\times10^{-3}T + 0.255\times10^{-6}T^2 - 21.700T^{-1}$

$\Delta Gf^\circ = -26.554 + 8.638\times10^{-3}T\ln T - 0.255\times10^{-6}T^2 - 10.850T^{-1} - 55.296\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

GaCl(g)

Gallium Monochloride (ideal gas)

[Formation: $Ga(c,l) + 0.5Cl_2(g) = GaCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.539	57.395	57.395	0	-16.860	-23.119	16.946
300	8.544	57.448	57.395	.016	-16.864	-23.158	16.870
302.9	8.549	57.530	57.396	.041	-16.869	-23.219	16.753
302.9	8.549	57.530	57.396	.041	-18.205	-23.219	16.753
400	8.729	59.935	57.735	.880	-18.410	-24.797	13.548
500	8.830	61.894	58.376	1.759	-18.601	-26.369	11.526
600	8.892	63.510	59.102	2.645	-18.789	-27.905	10.164
700	8.935	64.884	59.831	3.537	-18.972	-29.409	9.182
800	8.969	66.079	60.539	4.432	-19.155	-30.888	8.438
900	8.996	67.137	61.215	5.330	-19.337	-32.344	7.854
1000	9.019	68.087	61.856	6.231	-19.518	-33.780	7.383
1100	9.040	68.947	62.462	7.134	-19.698	-35.198	6.993
1200	9.060	69.734	63.035	8.039	-19.878	-36.599	6.665
1300	9.078	70.460	63.578	8.946	-20.057	-37.984	6.386
1400	9.096	71.134	64.095	9.855	-20.235	-39.358	6.144
1500	9.114	71.762	64.585	10.765	-20.413	-40.718	5.932
1600	9.131	72.351	65.053	11.677	-20.590	-42.066	5.746
1700	9.148	72.905	65.499	12.591	-20.766	-43.402	5.580
1800	9.165	73.428	65.924	13.507	-20.940	-44.728	5.431
1900	9.182	73.924	66.332	14.424	-21.114	-46.045	5.296
2000	9.200	74.396	66.725	15.343	-21.288	-47.354	5.174

Phase change: 302.9 K, melting point of Ga; $\Delta H° = 1.336$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.895 + 0.158\times10^{-3}T - 0.359\times10^{5}T^{-2}$

$H°- H°_{298} = 8.895\times10^{-3}T + 0.079\times10^{-6}T^2 + 0.359\times10^{2}T^{-1} - 2.779$

Formation equations (kcal/mol):

298.15-302.9 K: $\Delta Hf° = -16.259 - 2.014\times10^{-3}T - 0.065\times10^{-6}T^2 + 1.750T^{-1}$

$\Delta Gf° = -16.259 + 2.014\times10^{-3}T\ln T + 0.065\times10^{-6}T^2 + 0.875T^{-1} - 34.513\times10^{-3}T$

302.9-2000 K: $\Delta Hf° = -17.965 - 1.519\times10^{-3}T - 0.091\times10^{-6}T^2 + 68.950T^{-1}$

$\Delta Gf° = -17.965 + 1.519\times10^{-3}T\ln T + 0.091\times10^{-6}T^2 + 34.475T^{-1} - 26.422\times10^{-3}T$

Source: Data from Gurvich (95).

$GaCl_2(g)$

Gallium Dichloride (ideal gas)

[Formation: $Ga(c,l) + Cl_2(g) = GaCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.699	71.920	71.920	0	-57.660	-60.305	44.204
300	12.712	71.998	71.918	.024	-57.663	-60.321	43.943
302.9	12.726	72.120	71.919	.061	-57.669	-60.348	43.542
302.9	12.726	72.120	71.919	.061	-59.005	-60.348	43.542
400	13.178	75.727	72.424	1.321	-59.191	-60.750	33.192
500	13.423	78.696	73.392	2.652	-59.357	-61.118	26.715
600	13.564	81.157	74.487	4.002	-59.515	-61.456	22.385
700	13.653	83.255	75.594	5.363	-59.668	-61.767	19.284
800	13.711	85.082	76.668	6.731	-59.821	-62.058	16.953
900	13.752	86.700	77.694	8.105	-59.972	-62.327	15.135
1000	13.782	88.150	78.668	9.482	-60.124	-62.581	13.677
1100	13.804	89.465	79.591	10.861	-60.277	-62.820	12.481
1200	13.822	90.667	80.465	12.242	-60.431	-63.046	11.482
1300	13.838	91.774	81.293	13.625	-60.585	-63.257	10.634
1400	13.851	92.800	82.079	15.010	-60.739	-63.456	9.906
1500	13.865	93.756	82.826	16.395	-60.895	-63.646	9.273
1600	13.880	94.651	83.537	17.783	-61.050	-63.823	8.718
1700	13.895	95.493	84.216	19.171	-61.206	-63.991	8.226
1800	13.913	96.288	84.865	20.562	-61.361	-64.151	7.789
1900	13.933	97.041	85.486	21.954	-61.516	-64.301	7.396
2000	13.955	97.756	86.081	23.349	-61.671	-64.443	7.042

Phase change: 302.9 K, melting point of Ga; ΔH° = 1.336 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.764 + 0.104\times10^{-3}T - 0.974\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.764\times10^{-3}T + 0.052\times10^{-6}T^2 + 0.974\times10^{2}T^{-1} - 4.435$

Formation equations (kcal/mol):

298.15-302.9 K: $\Delta Hf^\circ = -57.281 - 1.559\times10^{-3}T - 0.136\times10^{-6}T^2 + 29.100T^{-1}$

$\Delta Gf^\circ = -57.281 + 1.559\times10^{-3}T\ln T + 0.136\times10^{-6}T^2 + 14.550T^{-1} - 19.231\times10^{-3}T$

302.9-2000 K: $\Delta Hf^\circ = -58.986 - 1.063\times10^{-3}T - 0.162\times10^{-6}T^2 + 96.300T^{-1}$

$\Delta Gf^\circ = -58.986 + 1.063\times10^{-3}T\ln T + 0.162\times10^{-6}T^2 + 48.150T^{-1} - 11.140\times10^{-3}T$

Source: Data from Gurvich (95).

$GaCl_3(g)$

Gallium Trichloride (ideal gas)

[Formation: $Ga(c,l) + 1.5Cl_2(g) = GaCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	17.909	77.686	77.686	0	-103.150	-99.570	72.986
300	17.929	77.797	77.687	.033	-103.152	-99.549	72.520
302.9	17.951	77.970	77.689	.085	-103.154	-99.514	71.801
302.9	17.951	77.970	77.689	.085	-104.490	-99.514	71.801
400	18.688	83.071	78.398	1.869	-104.555	-97.907	53.493
500	19.085	87.288	79.770	3.759	-104.589	-96.239	42.066
600	19.313	90.790	81.323	5.680	-104.611	-94.567	34.446
700	19.456	93.778	82.894	7.619	-104.624	-92.892	29.002
800	19.551	96.383	84.421	9.570	-104.638	-91.216	24.919
900	19.617	98.690	85.881	11.528	-104.650	-89.537	21.742
1000	19.664	100.759	87.267	13.492	-104.662	-87.859	19.201
1100	19.700	102.635	88.580	15.461	-104.673	-86.177	17.122
1200	19.727	104.350	89.823	17.432	-104.687	-84.496	15.389
1300	19.748	105.930	91.002	19.406	-104.701	-82.812	13.922
1400	19.765	107.394	92.122	21.381	-104.717	-81.128	12.665
1500	19.779	108.759	93.186	23.359	-104.733	-79.444	11.575
1600	19.790	110.035	94.199	25.337	-104.752	-77.756	10.621
1700	19.799	111.235	95.166	27.317	-104.771	-76.065	9.779
1800	19.807	112.367	96.091	29.297	-104.792	-74.378	9.031
1900	19.814	113.439	96.977	31.278	-104.814	-72.688	8.361
2000	19.819	114.455	97.825	33.260	-104.840	-70.996	7.758

Phase change: 302.9 K, melting point of Ga; ΔH° = 1.336 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.697 + 0.106\times10^{-3}T - 1.617\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.697\times10^{-3}T + 0.053\times10^{-6}T^2 + 1.617\times10^{2}T^{-1} - 6.420$

Formation equations (kcal/mol):

298.15-302.9 K: $\Delta Hf^\circ = -103.321 - 0.039\times10^{-3}T - 0.179\times10^{-6}T^2 + 59.250T^{-1}$

$\Delta Gf^\circ = -103.321 + 0.039\times10^{-3}T\ln T + 0.179\times10^{-6}T^2 + 29.625T^{-1} + 11.969\times10^{-3}T$

302.9-2000 K: $\Delta Hf^\circ = -105.027 + 0.457\times10^{-3}T - 0.205\times10^{-6}T^2 + 126.450T^{-1}$

$\Delta Gf^\circ = -105.027 - 0.457\times10^{-3}T\ln T + 0.205\times10^{-6}T^2 + 63.225T^{-1} + 20.060\times10^{-3}T$

Source: Data from Gurvich (95).

$(GaCl_3)_2(g)$

Dimeric Gallium Trichloride (ideal gas)

[Formation: $2Ga(c,l) + 3Cl_2(g) = (GaCl_3)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	39.430	119.628	119.628	0	-228.860	-211.043	154.697
300	39.475	119.872	119.629	.073	-228.856	-210.933	153.663
302.9	39.524	120.252	119.633	.188	-228.850	-210.761	152.067
302.9	39.524	120.252	119.633	.188	-231.522	-210.761	152.067
400	41.165	131.489	121.201	4.115	-231.294	-204.136	111.533
500	42.030	140.778	124.220	8.279	-230.977	-197.378	86.273
600	42.525	148.488	127.640	12.509	-230.632	-190.691	69.458
700	42.832	155.068	131.099	16.778	-230.269	-184.062	57.466
800	43.034	160.802	134.462	21.072	-229.903	-177.489	48.487
900	43.175	165.879	137.676	25.383	-229.532	-170.956	41.513
1000	43.277	170.434	140.728	29.706	-229.161	-164.471	35.945
1100	43.353	174.562	143.619	34.037	-228.791	-158.020	31.395
1200	43.410	178.337	146.357	38.376	-228.422	-151.604	27.611
1300	43.455	181.814	148.953	42.719	-228.055	-145.216	24.413
1400	43.491	185.035	151.416	47.066	-227.690	-138.859	21.677
1500	43.521	188.037	153.759	51.417	-227.327	-132.527	19.309
1600	43.544	190.846	155.990	55.770	-226.968	-126.218	17.240
1700	43.564	193.487	158.119	60.126	-226.609	-119.927	15.417
1800	43.581	195.977	160.153	64.483	-226.255	-113.665	13.801
1900	43.595	198.334	162.101	68.842	-225.902	-107.416	12.356
2000	43.607	200.571	163.970	73.202	-225.557	-101.191	11.057

Phase change: 302.9 K, melting point of Ga; $\Delta H° = 1.336$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 43.374 + 0.216\times10^{-3}T - 3.563\times10^{5}T^{-2}$

$H°- H°_{298} = 43.374\times10^{-3}T + 0.108\times10^{-6}T^2 + 3.563\times10^{2}T^{-1} - 14.137$

Formation equations (kcal/mol):

298.15-302.9 K: $\Delta Hf° = -230.499 + 3.901\times10^{-3}T - 0.356\times10^{-6}T^2 + 151.400T^{-1}$

$\Delta Gf° = -230.499 - 3.901\times10^{-3}T\ln T + 0.356\times10^{-6}T^2 + 75.700T^{-1} + 86.525\times10^{-3}T$

302.9-2000 K: $\Delta Hf° = -233.911 + 4.893\times10^{-3}T - 0.408\times10^{-6}T^2 + 285.800T^{-1}$

$\Delta Gf° = -233.911 - 4.893\times10^{-3}T\ln T + 0.408\times10^{-6}T^2 + 142.900T^{-1} + 102.707\times10^{-3}T$

Source: Data from Gurvich (95).

GaF(g)

Gallium Monofluoride (ideal gas)

[Formation: $Ga(c,l) + 0.5F_2(g) = GaF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	7.974	54.422	54.422	0	-55.600	-61.695	45.223
300	7.982	54.472	54.422	.015	-55.604	-61.733	44.972
302.9	7.992	54.549	54.423	.038	-55.611	-61.793	44.585
302.9	7.992	54.549	54.423	.038	-56.947	-61.793	44.585
400	8.330	56.820	54.740	.832	-57.166	-63.312	34.592
500	8.542	58.703	55.351	1.676	-57.368	-64.825	28.335
600	8.678	60.273	56.043	2.538	-57.561	-66.297	24.149
700	8.770	61.619	56.748	3.410	-57.749	-67.740	21.149
800	8.837	62.794	57.430	4.291	-57.933	-69.153	18.892
900	8.887	63.838	58.086	5.177	-58.118	-70.545	17.130
1000	8.928	64.777	58.709	6.068	-58.302	-71.916	15.717
1100	8.962	65.629	59.300	6.962	-58.486	-73.269	14.557
1200	8.990	66.410	59.860	7.860	-58.668	-74.605	13.587
1300	9.016	67.131	60.392	8.761	-58.850	-75.924	12.764
1400	9.039	67.800	60.898	9.663	-59.033	-77.233	12.056
1500	9.061	68.424	61.379	10.568	-59.214	-78.526	11.441
1600	9.081	69.010	61.838	11.475	-59.396	-79.808	10.901
1700	9.101	69.561	62.276	12.385	-59.575	-81.077	10.423
1800	9.120	70.082	62.696	13.295	-59.756	-82.338	9.997
1900	9.138	70.575	63.097	14.208	-59.934	-83.587	9.615
2000	9.156	71.044	63.482	15.123	-60.112	-84.826	9.269

Phase change: 302.9 K, melting point of Ga; ΔH° = 1.336 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.723 + 0.254\times10^{-3}T - 0.733\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.723\times10^{-3}T + 0.127\times10^{-6}T^2 + 0.733\times10^{2}T^{-1} - 2.858$

Formation equations (kcal/mol):

298.15-302.9 K: $\Delta Hf^\circ = -55.068 - 2.027\times10^{-3}T - 0.060\times10^{-6}T^2 + 23.050T^{-1}$

$\Delta Gf^\circ = -55.068 + 2.027\times10^{-3}T\ln T + 0.060\times10^{-6}T^2 + 11.525T^{-1} - 33.925\times10^{-3}T$

302.9-2000 K: $\Delta Hf^\circ = -56.773 - 1.531\times10^{-3}T - 0.086\times10^{-6}T^2 + 90.250T^{-1}$

$\Delta Gf^\circ = -56.773 + 1.531\times10^{-3}T\ln T + 0.086\times10^{-6}T^2 + 45.125T^{-1} - 25.834\times10^{-3}T$

Source: Data from Gurvich (95).

$GaF_2(g)$

Gallium Difluoride (ideal gas)

[Formation: $Ga(c,l) + F_2(g) = GaF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	11.350	66.776	66.776	0	-128.300	-130.857	95.919
300	11.368	66.846	66.776	.021	-128.305	-130.873	95.340
302.9	11.391	66.955	66.777	.054	-128.313	-130.898	94.445
302.9	11.391	66.955	66.777	.054	-129.649	-130.898	94.445
400	12.155	70.232	67.232	1.200	-129.890	-131.261	71.717
500	12.661	73.003	68.117	2.443	-130.095	-131.578	57.512
600	12.989	75.342	69.132	3.726	-130.281	-131.858	48.029
700	13.207	77.362	70.166	5.037	-130.454	-132.106	41.245
800	13.358	79.136	71.180	6.365	-130.623	-132.332	36.151
900	13.467	80.716	72.153	7.707	-130.787	-132.534	32.183
1000	13.546	82.139	73.081	9.058	-130.951	-132.720	29.006
1100	13.607	83.433	73.964	10.416	-131.114	-132.888	26.402
1200	13.653	84.619	74.803	11.779	-131.277	-133.043	24.230
1300	13.690	85.714	75.602	13.146	-131.440	-133.183	22.390
1400	13.720	86.729	76.360	14.517	-131.604	-133.312	20.811
1500	13.744	87.677	77.084	15.890	-131.769	-133.430	19.440
1600	13.764	88.564	77.773	17.265	-131.935	-133.533	18.240
1700	13.781	89.399	78.433	18.642	-132.101	-133.628	17.179
1800	13.795	90.187	79.064	20.021	-132.269	-133.713	16.235
1900	13.809	90.934	79.670	21.402	-132.436	-133.789	15.389
2000	13.820	91.642	80.250	22.783	-132.607	-133.855	14.627

Phase change: 302.9 K, melting point of Ga; $\Delta H° = 1.336$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.198 + 0.440\times10^{-3}T - 1.759\times10^{5}T^{-2}$

$H°- H°_{298} = 13.198\times10^{-3}T + 0.220\times10^{-6}T^2 + 1.759\times10^{2}T^{-1} - 4.545$

Formation equations (kcal/mol):

298.15-302.9 K: $\Delta Hf° = -128.010 - 1.806\times10^{-3}T - 0.054\times10^{-6}T^2 + 75.400T^{-1}$

$\Delta Gf° = -128.010 + 1.806\times10^{-3}T\ln T + 0.054\times10^{-6}T^2 + 37.700T^{-1} - 20.279\times10^{-3}T$

302.9-2000 K: $\Delta Hf° = -129.715 - 1.310\times10^{-3}T - 0.080\times10^{-6}T^2 + 142.600T^{-1}$

$\Delta Gf° = -129.715 + 1.310\times10^{-3}T\ln T + 0.080\times10^{-6}T^2 + 71.300T^{-1} - 12.188\times10^{-3}T$

Source: Data from Gurvich (95).

GaF_3(c)

Gallium Trifluoride

[Formation: $Ga(c,l) + 1.5F_2(g) = GaF_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	21.272	22.945	22.945	0	-280.800	-263.067	192.831
300	21.288	23.076	22.946	.039	-280.794	-262.958	191.562
302.9	21.314	23.281	22.948	.101	-280.784	-262.786	189.604
302.9	21.314	23.281	22.948	.101	-282.120	-262.786	189.604
400	22.183	29.323	23.791	2.213	-281.768	-256.636	140.217
500	23.078	34.369	25.417	4.476	-281.355	-250.398	109.448
600	23.973	38.656	27.276	6.828	-280.887	-244.251	88.967
700	24.868	42.419	29.175	9.271	-280.352	-238.185	74.364
800	25.763	45.797	31.045	11.802	-279.749	-232.202	63.434
900	26.658	48.884	32.858	14.423	-279.070	-226.298	54.952
1000	27.552	51.739	34.605	17.134	-278.314	-220.475	48.184
1100	28.447	54.407	36.285	19.934	-277.478	-214.731	42.663
1200	29.342	56.920	37.901	22.823	-276.560	-209.067	38.076
1300	30.237	59.304	39.456	25.802	-275.559	-203.480	34.208
1400	31.132	61.577	40.955	28.871	-274.475	-197.978	30.905
1500	32.027	63.756	42.404	32.028	-273.307	-192.556	28.055
1600	32.922	65.851	43.803	35.276	-272.053	-187.210	25.571
1700	33.816	67.874	45.160	38.613	-270.714	-181.947	23.391
1800	34.712	69.832	46.477	42.039	-269.290	-176.767	21.462
1900	35.606	71.733	47.757	45.555	-267.779	-171.667	19.746
2000	36.501	73.582	49.002	49.160	-266.184	-166.650	18.210

Phase change: 302.9 K, melting point of Ga; $\Delta H° = 1.336$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 18.606 + 8.946\times10^{-3}T - 0.001\times10^{5}T^{-2}$

$H°-H°_{298} = 18.606\times10^{-3}T + 4.473\times10^{-6}T^2 + 0.001\times10^{2}T^{-1} - 5.945$

Formation equations (kcal/mol):

298.15-302.9 K: $\Delta Hf° = -280.466 - 0.652\times10^{-3}T + 4.112\times10^{-6}T^2 - 150.650T^{-1}$

$\Delta Gf° = -280.466 + 0.652\times10^{-3}T\ln T - 4.112\times10^{-6}T^2 - 75.325T^{-1} + 56.715\times10^{-3}T$

302.9-2000 K: $\Delta Hf° = -282.172 - 0.156\times10^{-3}T + 4.086\times10^{-6}T^2 - 83.450T^{-1}$

$\Delta Gf° = -282.172 + 0.156\times10^{-3}T\ln T - 4.086\times10^{-6}T^2 - 41.725T^{-1} + 64.806\times10^{-3}T$

Source: Data from Gurvich (95).

$GaF_3(g)$

Gallium Trifluoride (ideal gas)

[Formation: $Ga(c,l) + 1.5F_2(g) = GaF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	15.766	69.990	69.990	0	-220.250	-216.543	158.728
300	15.795	70.087	69.990	.029	-220.254	-216.521	157.733
302.9	15.832	70.239	69.992	.075	-220.260	-216.485	156.198
302.9	15.832	70.239	69.992	.075	-221.596	-216.485	156.198
400	17.088	74.822	70.627	1.678	-221.754	-214.820	117.371
500	17.901	78.729	71.867	3.431	-221.850	-213.073	93.133
600	18.421	82.043	73.295	5.249	-221.917	-211.312	76.970
700	18.767	84.910	74.754	7.109	-221.965	-209.541	65.421
800	19.005	87.432	76.183	8.999	-222.003	-207.763	56.758
900	19.176	89.681	77.561	10.908	-222.035	-205.980	50.018
1000	19.301	91.708	78.876	12.832	-222.066	-204.196	44.627
1100	19.396	93.553	80.128	14.767	-222.095	-202.408	40.214
1200	19.469	95.244	81.318	16.711	-222.122	-200.618	36.537
1300	19.527	96.804	82.449	18.661	-222.150	-198.822	33.425
1400	19.573	98.253	83.527	20.616	-222.180	-197.029	30.757
1500	19.611	99.605	84.555	22.575	-222.211	-195.232	28.445
1600	19.642	100.872	85.536	24.538	-222.242	-193.432	26.421
1700	19.668	102.063	86.473	26.503	-222.273	-191.628	24.635
1800	19.689	103.188	87.371	28.471	-222.309	-189.826	23.048
1900	19.708	104.253	88.231	30.441	-222.343	-188.019	21.627
2000	19.724	105.264	89.058	32.413	-222.382	-186.212	20.348

Phase change: 302.9 K, melting point of Ga; $\Delta H° = 1.336$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 18.902 + 0.564\times10^{-3}T - 2.937\times10^{5}T^{-2}$

$H°- H°_{298} = 18.902\times10^{-3}T + 0.282\times10^{-6}T^2 + 2.937\times10^{2}T^{-1} - 6.646$

Formation equations (kcal/mol):

298.15-302.9 K: $\Delta Hf° = -220.616 - 0.356\times10^{-3}T - 0.079\times10^{-6}T^2 + 142.950T^{-1}$

$\Delta Gf° = -220.616 + 0.356\times10^{-3}T\ln T + 0.079\times10^{-6}T^2 + 71.475T^{-1} + 10.805\times10^{-3}T$

302.9-2000 K: $\Delta Hf° = -222.322 + 0.140\times10^{-3}T - 0.105\times10^{-6}T^2 + 210.150T^{-1}$

$\Delta Gf° = -222.322 - 0.140\times10^{-3}T\ln T + 0.105\times10^{-6}T^2 + 105.075T^{-1} + 18.896\times10^{-3}T$

Source: Data from Gurvich (95).

$GdBr_3(c,l)$

Gadolinium Tribromide

[Formation: $Gd(c) + 1.5Br_2(l,g) = GdBr_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	23.200	45.400	45.400	0	-198.100	-190.524	139.656
300	23.227	45.544	45.401	.043	-198.123	-190.478	138.761
332.6	23.520	47.955	45.535	.805	-198.519	-189.627	124.601
332.6	23.520	47.955	45.535	.805	-209.116	-189.627	124.601
400	24.125	52.365	46.325	2.416	-208.850	-185.713	101.468
500	24.517	57.796	48.094	4.851	-208.411	-179.981	78.668
600	24.720	62.285	50.095	7.314	-207.966	-174.323	63.496
700	24.878	66.108	52.118	9.793	-207.532	-168.751	52.686
800	25.076	69.442	54.078	12.291	-207.104	-163.238	44.594
900	25.378	72.412	55.954	14.812	-206.678	-157.782	38.314
1000	25.836	75.108	57.737	17.371	-206.236	-152.381	33.302
1058	26.192	76.574	58.729	18.880	-205.965	-149.253	30.831
1058	33.300	85.189	58.729	27.995	-196.850	-149.253	30.831
1100	33.300	86.486	59.764	29.394	-196.353	-147.373	29.280
1200	33.300	89.383	62.113	32.724	-195.190	-142.979	26.040
1300	33.300	92.048	64.314	36.054	-194.055	-138.675	23.313

*Entropy and heat capacity at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
1058 K, melting point of $GdBr_3$; ΔH° = 9.115 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1058 K: $Cp^\circ = 24.366 + 1.376\times10^{-3}T - 1.425\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 24.366\times10^{-3}T + 0.688\times10^{-6}T^2 + 1.425\times10^{2}T^{-1} - 7.804$

1058-1300 K: $Cp^\circ = 33.300$

$H^\circ - H^\circ_{298} = 33.300\times10^{-3}T - 7.236$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -198.219 - 5.556\times10^{-3}T - 1.365\times10^{-6}T^2 + 565.600T^{-1}$

$\Delta Gf^\circ = -198.219 + 5.556\times10^{-3}T\ln T + 1.365\times10^{-6}T^2 + 282.800T^{-1} - 9.439\times10^{-3}T$

332.6-1058 K: $\Delta Hf^\circ = -213.220 + 8.185\times10^{-3}T - 1.598\times10^{-6}T^2 + 518.500T^{-1}$

$\Delta Gf^\circ = -213.220 - 8.185\times10^{-3}T\ln T + 1.598\times10^{-6}T^2 + 259.250T^{-1} + 115.593\times10^{-3}T$

1058-1300 K: $\Delta Hf^\circ = -212.652 + 17.119\times10^{-3}T - 2.286\times10^{-6}T^2 + 376.000T^{-1}$

$\Delta Gf^\circ = -212.652 - 17.119\times10^{-3}T\ln T + 2.286\times10^{-6}T^2 + 188.000T^{-1} + 176.610\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Hurtgen (103). Entropy and heat capacity at 298 K estimated. High-temperature data based on Dworkin (69).

$GdBr_3(g)$

Gadolinium Tribromide (ideal gas)

[Formation: $Gd(c,l) + 1.5Br_2(l,g) = GdBr_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	19.103	95.321	95.321	0	-127.000	-134.308	98.449
300	19.112	95.439	95.322	.035	-127.030	-134.354	97.876
332.6	19.216	97.416	95.432	.660	-127.564	-135.123	88.787
332.6	19.216	97.416	95.432	.660	-138.162	-135.123	88.787
400	19.431	100.987	96.075	1.965	-138.201	-134.513	73.494
500	19.585	105.341	97.509	3.916	-138.245	-133.588	58.391
600	19.671	108.920	99.120	5.880	-138.299	-132.638	48.313
700	19.724	111.957	100.744	7.849	-138.376	-131.689	41.115
800	19.758	114.593	102.313	9.824	-138.471	-130.726	35.712
900	19.782	116.922	103.810	11.801	-138.589	-129.752	31.508
1000	19.799	119.007	105.227	13.780	-138.727	-128.771	28.143
1100	19.812	120.894	106.567	15.760	-138.887	-127.756	25.382
1200	19.821	122.619	107.834	17.742	-139.072	-126.744	23.083
1300	19.829	124.206	109.033	19.725	-139.284	-125.709	21.133
1400	19.835	125.675	110.169	21.708	-139.527	-124.644	19.457
1500	19.839	127.044	111.250	23.691	-139.803	-123.571	18.004
1533	19.840	127.476	111.595	24.346	-139.903	-123.215	17.566
1533	19.840	127.476	111.595	24.346	-140.838	-123.215	17.566
1585	19.842	128.137	112.126	25.378	-140.870	-122.623	16.908
1585	19.842	128.137	112.126	25.378	-143.273	-122.623	16.908
1600	19.843	128.324	112.277	25.676	-143.313	-122.430	16.723
1700	19.847	129.528	113.257	27.660	-143.582	-121.118	15.571
1800	19.849	130.662	114.193	29.645	-143.851	-119.782	14.543
1900	19.852	131.735	115.088	31.630	-144.122	-118.435	13.623
2000	19.854	132.754	115.946	33.615	-144.396	-117.091	12.795

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
1533 K, α - β transition point of Gd; ΔH° = 0.935 kcal/mol.
1585 K, melting point of Gd: ΔH° = 2.403 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.846 + 0.016\times10^{-3}T - 0.665\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.846\times10^{-3}T + 0.008\times10^{-6}T^2 + 0.665\times10^{2}T^{-1} - 6.141$

$GdBr_3(g)$ - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -125.456 - 10.076\times10^{-3}T - 2.045\times10^{-6}T^2 + 489.600T^{-1}$

$\Delta Gf^\circ = -125.456 + 10.076\times10^{-3}T\ln T + 2.045\times10^{-6}T^2 + 244.800T^{-1} - 90.466\times10^{-3}T$

332.6-1533 K: $\Delta Hf^\circ = -140.457 + 3.665\times10^{-3}T - 2.278\times10^{-6}T^2 + 442.500T^{-1}$

$\Delta Gf^\circ = -140.457 - 3.665\times10^{-3}T\ln T + 2.278\times10^{-6}T^2 + 221.250T^{-1} + 34.566\times10^{-3}T$

1533-1585 K: $\Delta Hf^\circ = -140.098 - 0.376\times10^{-3}T - 0.075\times10^{-6}T^2 + 19.400T^{-1}$

$\Delta Gf^\circ = -140.098 + 0.376\times10^{-3}T\ln T + 0.075\times10^{-6}T^2 + 9.700T^{-1} + 8.159\times10^{-3}T$

1585-2000 K: $\Delta Hf^\circ = -139.247 - 2.429\times10^{-3}T - 0.075\times10^{-6}T^2 + 19.400T^{-1}$

$\Delta Gf^\circ = -139.247 + 2.429\times10^{-3}T\ln T + 0.075\times10^{-6}T^2 + 9.700T^{-1} - 7.505\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

$GdCl_3$(c,l)

Gadolinium Trichloride

[Formation: $Gd(c) + 1.5Cl_2(g) = GdCl_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	23.370	36.190	36.190	0	-241.000	-223.115	163.546
300	23.395	36.335	36.192	.043	-240.995	-223.006	162.458
400	24.332	43.205	37.120	2.434	-240.587	-217.070	118.600
500	24.979	48.707	38.907	4.900	-240.073	-211.250	92.336
600	25.588	53.314	40.934	7.428	-239.535	-205.523	74.861
700	26.250	57.307	42.993	10.020	-238.965	-199.897	62.410
800	27.002	60.860	45.009	12.681	-238.361	-194.359	53.096
875	27.637	63.308	46.474	14.730	-237.871	-190.255	47.520
875	33.300	74.428	46.474	24.460	-228.141	-190.255	47.520
900	33.300	75.366	47.264	25.292	-227.832	-189.177	45.938
1000	33.300	78.874	50.252	28.622	-226.610	-184.957	40.422
1100	33.300	82.048	53.001	31.952	-225.412	-180.838	35.929
1200	33.300	84.946	55.544	35.282	-224.244	-176.846	32.208
1300	33.300	87.611	57.909	38.612	-223.105	-172.943	29.074

Phase change: 875 K melting point of $GdCl_3$; ΔH° = 9.730 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-875 K: $Cp^\circ = 22.251 + 5.986\times10^{-3}T - 0.592\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 22.251\times10^{-3}T + 2.993\times10^{-6}T^2 + 0.592\times10^{2}T^{-1} - 7.099$

875-1300 K: $Cp^\circ = 33.300$

$H^\circ - H^\circ_{298} = 33.300\times10^{-3}T - 4.678$

Formation equations (kcal/mol):

298.15-875 K: $\Delta Hf^\circ = -244.188 + 6.225\times10^{-3}T + 0.658\times10^{-6}T^2 + 379.850T^{-1}$

$\Delta Gf^\circ = -244.188 - 6.225\times10^{-3}T\ln T - 0.658\times10^{-6}T^2 + 189.925T^{-1} + 104.203\times10^{-3}T$

875-1300 K: $\Delta Hf^\circ = -241.767 + 17.273\times10^{-3}T - 2.335\times10^{-6}T^2 + 320.650T^{-1}$

$\Delta Gf^\circ = -241.767 - 17.273\times10^{-3}T\ln T + 2.335\times10^{-6}T^2 + 160.325T^{-1} + 173.704\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (207). Low-temperature heat capacities and entropy at 298 K from Sommers (226). High-temperature data based on Dworkin (69).

$GdCl_3(g)$

Gadolinium Trichloride (ideal gas)

[Formation: $Gd(c,l) + 1.5Cl_3(g) = GdCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.691	88.760	88.760	0	-166.500	-164.289	120.426
300	18.704	88.876	88.760	.035	-166.503	-164.276	119.674
400	19.182	94.331	89.501	1.932	-166.589	-163.522	89.343
500	19.420	98.639	90.913	3.863	-166.610	-162.753	71.138
600	19.554	102.193	92.506	5.812	-166.650	-161.967	58.996
700	19.636	105.214	94.111	7.772	-166.714	-161.180	50.322
800	19.691	107.840	95.666	9.739	-166.803	-160.385	43.815
900	19.728	110.161	97.150	11.710	-166.913	-159.574	38.749
1000	19.755	112.241	98.557	13.684	-167.048	-158.761	34.697
1100	19.775	114.125	99.888	15.661	-167.203	-157.914	31.374
1200	19.791	115.847	101.148	17.639	-167.387	-157.071	28.606
1300	19.803	117.431	102.339	19.619	-167.598	-156.202	26.260
1400	19.812	118.899	103.471	21.599	-167.841	-155.307	24.244
1500	19.820	120.266	104.545	23.581	-168.115	-154.400	22.496
1533	19.822	120.697	104.888	24.235	-168.215	-154.099	21.969
1533	19.822	120.697	104.888	24.235	-169.150	-154.099	21.969
1585	19.825	121.359	105.419	25.266	-169.183	-153.598	21.179
1585	19.825	121.359	105.419	25.266	-171.586	-153.598	21.179
1600	19.826	121.546	105.569	25.563	-171.626	-153.430	20.957
1700	19.831	122.748	106.544	27.546	-171.895	-152.279	19.577
1800	19.836	123.881	107.475	29.530	-172.165	-151.113	18.347
1900	19.839	124.954	108.368	31.513	-172.438	-149.935	17.246
2000	19.843	125.972	109.224	33.497	-172.715	-148.757	16.255

Phase changes: 1533 K, α - β transition point of Gd; $\Delta H°$ = 0.935 kcal/mol.
1585 K, melting point of Gd: $\Delta H°$ = 2.403 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.804 + 0.042\times10^{-3}T - 1.001\times10^{5}T^{-2}$

$H°- H°_{298} = 19.804\times10^{-3}T + 0.021\times10^{-6}T^2 + 1.001\times10^{2}T^{-1} - 6.242$

Formation equations (kcal/mol):

298.15-1533 K: $\Delta Hf° = -168.832 + 3.778\times10^{-3}T - 2.314\times10^{-6}T^2 + 420.750T^{-1}$

$\Delta Gf° = -168.832 - 3.778\times10^{-3}T\ln T + 2.314\times10^{-6}T^2 + 210.375T^{-1} + 33.702\times10^{-3}T$

1533-1585 K: $\Delta Hf° = -168.473 - 0.263\times10^{-3}T - 0.111\times10^{-6}T^2 - 2.350T^{-1}$

$\Delta Gf° = -168.473 + 0.263\times10^{-3}T\ln T + 0.111\times10^{-6}T^2 - 1.175T^{-1} + 7.295\times10^{-3}T$

1585-2000 K: $\Delta Hf° = -167.622 - 2.316\times10^{-3}T - 0.111\times10^{-6}T^2 - 2.350T^{-1}$

$\Delta Gf° = -167.622 + 2.316\times10^{-3}T\ln T + 0.111\times10^{-6}T^2 - 1.175T^{-1} - 8.370\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (167). Other data based on Myers (165) and Dieke (56).

$GdF_3(c,l)$

Gadolinium Trifluoride

[Formation: $Gd(c,l) + 1.5F_2(g) = GdF_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	21.126	27.431	27.431	0	-406.100	-387.772	284.241
300	21.176	27.562	27.432	.039	-406.098	-387.660	282.406
400	22.962	33.932	28.287	2.258	-405.770	-381.558	208.471
500	23.853	39.161	29.955	4.603	-405.303	-375.559	164.155
600	24.394	43.561	31.866	7.017	-404.820	-369.645	134.641
700	24.776	47.352	33.815	9.476	-404.340	-363.819	113.588
800	25.077	50.680	35.719	11.969	-403.867	-358.064	97.817
900	25.336	53.649	37.549	14.490	-403.399	-352.365	85.565
1000	25.572	56.331	39.295	17.036	-402.940	-346.729	75.776
1100	25.797	58.779	40.957	19.604	-402.488	-341.118	67.773
1200	26.018	61.033	42.537	22.195	-402.046	-335.566	61.114
1300	26.238	63.124	44.041	24.808	-401.613	-330.043	55.485
1348	26.345	64.077	44.737	26.070	-401.410	-327.404	53.081
1348	31.275	65.142	44.737	27.505	-399.975	-327.404	53.081
1400	31.275	66.326	45.517	29.132	-399.506	-324.605	50.672
1500	31.275	68.484	46.978	32.259	-398.630	-319.284	46.519
1505	31.275	68.588	47.050	32.415	-398.588	-319.021	46.326
1505	30.550	76.914	47.050	44.945	-386.058	-319.021	46.326
1533	30.550	77.477	47.601	45.800	-385.842	-317.777	45.303
1533	30.550	77.477	47.601	45.800	-386.777	-317.777	45.303
1585	30.550	78.496	48.598	47.389	-386.251	-315.454	43.496
1585	30.550	78.496	48.598	47.389	-388.654	-315.454	43.496
1600	30.550	78.784	48.880	47.847	-388.533	-314.765	42.994
1700	30.550	80.636	50.694	50.902	-387.728	-310.174	39.875
1800	30.550	82.382	52.406	53.957	-386.928	-305.631	37.108

Phase changes: 1348 K, α - β transition point of GdF_3; ΔH° = 1.435 kcal/mol.
1505 K, melting point of GdF_3; ΔH° = 12.530 kcal/mol.
1533 K, α - β transition point of Gd; ΔH° = 0.935 kcal/mol.
1585 K, melting point of Gd: ΔH° = 2.403 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1348 K: $Cp^\circ = 24.376 + 1.552\times10^{-3}T - 3.300\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 24.376\times10^{-3}T + 0.776\times10^{-6}T^2 + 3.300\times10^{2}T^{-1} - 8.444$

1348-1505 K: $Cp^\circ = 31.275$

$H^\circ - H^\circ_{298} = 31.275\times10^{-3}T - 14.654$

1505-1800 K: $Cp^\circ = 30.550$

$H^\circ - H^\circ_{298} = 30.550\times10^{-3}T - 1.033$

GdF_3(c,1) - Continued

Formation equations (kcal/mol):

298.15-1348 K: $\Delta Hf^\circ = -410.602 + 8.828\times10^{-3}T - 1.688\times10^{-6}T^2 + 602.350T^{-1}$

$\Delta Gf^\circ = -410.602 - 8.828\times10^{-3}T\ln T + 1.688\times10^{-6}T^2 + 301.175T^{-1} + 122.981\times10^{-3}T$

1348-1505 K: $\Delta Hf^\circ = -416.812 + 15.727\times10^{-3}T - 2.464\times10^{-6}T^2 + 272.350T^{-1}$

$\Delta Gf^\circ = -416.812 - 15.727\times10^{-3}T\ln T + 2.464\times10^{-6}T^2 + 136.175T^{-1} + 176.350\times10^{-3}T$

1505-1533 K: $\Delta Hf^\circ = -403.191 + 15.002\times10^{-3}T - 2.464\times10^{-6}T^2 + 272.350T^{-1}$

$\Delta Gf^\circ = -403.191 - 15.002\times10^{-3}T\ln T + 2.464\times10^{-6}T^2 + 136.175T^{-1} + 161.995\times10^{-3}T$

1533-1585 K: $\Delta Hf^\circ = -402.833 + 10.961\times10^{-3}T - 0.261\times10^{-6}T^2 - 150.750T^{-1}$

$\Delta Gf^\circ = -402.833 - 10.961\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 - 75.375T^{-1} + 135.587\times10^{-3}T$

1585-1800 K: $\Delta Hf^\circ = -401.982 + 8.908\times10^{-3}T - 0.261\times10^{-6}T^2 - 150.750T^{-1}$

$\Delta Gf^\circ = -401.982 - 8.908\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 - 75.375T^{-1} + 119.923\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Johnson (111). Low-temperature heat capacities and entropy at 298 K from Flotow (81). High-temperature data based on Spedding (222).

$GdF_3(g)$

Gadolinium Trifluoride (ideal gas)

[Formation: $Gd(c,l) + 1.5F_2(g) = GdF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	17.095	80.122	80.122	0	-298.000	-295.381	216.518
300	17.120	80.228	80.122	.032	-298.005	-295.366	215.171
400	18.114	85.303	80.808	1.798	-298.129	-294.467	160.887
500	18.674	89.411	82.131	3.640	-298.166	-293.547	128.308
600	19.010	92.848	83.638	5.526	-298.211	-292.608	106.581
700	19.225	95.796	85.170	7.438	-298.278	-291.668	91.062
800	19.369	98.373	86.663	9.368	-298.367	-290.719	79.420
900	19.471	100.660	88.092	11.311	-298.478	-289.754	70.361
1000	19.545	102.716	89.454	13.262	-298.614	-288.788	63.114
1100	19.600	104.581	90.746	15.219	-298.773	-287.785	57.177
1200	19.643	106.289	91.972	17.181	-298.960	-286.787	52.230
1300	19.676	107.862	93.134	19.147	-299.174	-285.763	48.041
1400	19.703	109.321	94.238	21.116	-299.422	-284.714	44.445
1500	19.724	110.681	95.289	23.088	-299.701	-283.651	41.327
1533	19.730	111.110	95.625	23.739	-299.803	-283.298	40.387
1533	19.730	111.110	95.625	23.739	-300.738	-283.298	40.387
1585	19.739	111.769	96.145	24.765	-300.775	-282.715	38.982
1585	19.739	111.769	96.145	24.765	-303.178	-282.715	38.982
1600	19.742	111.955	96.292	25.061	-303.219	-282.524	38.590
1700	19.756	113.152	97.248	27.036	-303.493	-281.218	36.153
1800	19.769	114.282	98.164	29.012	-303.773	-279.896	33.984
1900	19.779	115.351	99.041	30.989	-304.054	-278.562	32.041
2000	19.788	116.366	99.882	32.968	-304.339	-277.225	30.293

Phase changes: 1533 K, α - β transition point of Gd; ΔH° = 0.935 kcal/mol.
1585 K, melting point of Gd: ΔH° = 2.403 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.476 + 0.230\times10^{-3}T - 2.178\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.476\times10^{-3}T + 0.115\times10^{-6}T^2 + 2.178\times10^{2}T^{-1} - 6.547$

Formation equations (kcal/mol):

298.15-1533 K: $\Delta Hf^\circ = -300.606 + 3.928\times10^{-3}T - 2.349\times10^{-6}T^2 + 490.150T^{-1}$

$\Delta Gf^\circ = -300.606 - 3.928\times10^{-3}T\ln T + 2.349\times10^{-6}T^2 + 245.075T^{-1} + 36.447\times10^{-3}T$

1533-1585 K: $\Delta Hf^\circ = -300.248 - 0.113\times10^{-3}T - 0.146\times10^{-6}T^2 + 67.050T^{-1}$

$\Delta Gf^\circ = -300.248 + 0.113\times10^{-3}T\ln T + 0.146\times10^{-6}T^2 + 33.525T^{-1} + 10.040\times10^{-3}T$

1585-2000 K: $\Delta Hf^\circ = -299.397 - 2.166\times10^{-3}T - 0.146\times10^{-6}T^2 + 67.050T^{-1}$

$\Delta Gf^\circ = -299.397 + 2.166\times10^{-3}T\ln T + 0.146\times10^{-6}T^2 + 33.525T^{-1} - 5.624\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

GdI_3(c,l)

Gadolinium Triiodide

[Formation: $Gd(c) + 1.5I_2(c,l,g) = GdI_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	23.600	54.100	54.100	0	-142.000	-140.874	103.262
300	23.625	54.246	54.100	.044	-142.008	-140.867	102.620
386.8	24.361	60.353	54.844	2.131	-142.380	-140.494	79.381
386.8	24.361	60.353	54.844	2.131	-147.943	-140.494	79.381
400	24.473	61.172	55.040	2.453	-148.094	-140.238	76.621
458.4	24.715	64.529	56.038	3.892	-148.735	-139.042	66.290
458.4	24.715	64.529	56.038	3.892	-163.766	-139.042	66.290
500	24.887	66.683	56.835	4.924	-163.573	-136.805	59.797
600	25.122	71.243	58.868	7.425	-163.104	-131.485	47.893
700	25.272	75.127	60.920	9.945	-162.638	-126.250	39.417
800	25.376	78.509	62.912	12.478	-162.184	-121.082	33.078
900	25.455	81.503	64.814	15.020	-161.745	-115.972	28.161
1000	25.516	84.188	66.620	17.568	-161.321	-110.917	24.240
1013	25.524	84.518	66.848	17.900	-161.267	-110.262	23.788
1013	30.550	84.735	66.848	18.120	-161.047	-110.262	23.788
1100	30.550	87.252	68.363	20.778	-160.258	-105.922	21.045
1200	30.550	89.910	70.049	23.833	-159.379	-101.029	18.400
1204	30.550	90.012	70.116	23.955	-159.345	-100.835	18.303
1204	37.250	100.730	70.116	36.860	-146.440	-100.835	18.303
1300	37.250	103.588	72.483	40.436	-144.978	-97.256	16.350

*Entropy and heat capacity at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
1013 K, α - β transition point of GdI_3; ΔH° = 0.220 kcal/mol.
1204 K, melting point of GdI_3; ΔH° = 12.905 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1013 K: $Cp^\circ = 25.483 + 0.208\times10^{-3}T - 1.750\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.483\times10^{-3}T + 0.104\times10^{-6}T^2 + 1.750\times10^{2}T^{-1} - 8.194$

1013-1204 K: $Cp^\circ = 30.550$

$H^\circ - H^\circ_{298} = 30.550\times10^{-3}T - 12.827$

1204-1300 K: $Cp^\circ = 37.250$

$H^\circ - H^\circ_{298} = 37.250\times10^{-3}T - 7.989$

$GdI_3(c,l)$ - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -144.629 + 3.382\times10^{-3}T - 4.337\times10^{-6}T^2 + 598.100T^{-1}$

$\Delta Gf^\circ = -144.629 - 3.382\times10^{-3}T\ln T + 4.337\times10^{-6}T^2 + 299.050T^{-1} + 27.203\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -146.811 - 6.225\times10^{-3}T - 2.099\times10^{-6}T^2 + 598.100T^{-1}$

$\Delta Gf^\circ = -146.811 + 6.225\times10^{-3}T\ln T + 2.099\times10^{-6}T^2 + 299.050T^{-1} - 23.520\times10^{-3}T$

458.4-1013 K: $\Delta Hf^\circ = -168.881 + 9.286\times10^{-3}T - 2.201\times10^{-6}T^2 + 575.150T^{-1}$

$\Delta Gf^\circ = -168.881 - 9.286\times10^{-3}T\ln T + 2.201\times10^{-6}T^2 + 287.575T^{-1} + 119.674\times10^{-3}T$

1013-1204 K: $\Delta Hf^\circ = -173.515 + 14.353\times10^{-3}T - 2.305\times10^{-6}T^2 + 400.150T^{-1}$

$\Delta Gf^\circ = -173.515 - 14.353\times10^{-3}T\ln T + 2.305\times10^{-6}T^2 + 200.075T^{-1} + 159.295\times10^{-3}T$

1204-1300 K: $\Delta Hf^\circ = -168.676 + 21.053\times10^{-3}T - 2.305\times10^{-6}T^2 + 400.150T^{-1}$

$\Delta Gf^\circ = -168.676 - 21.053\times10^{-3}T\ln T + 2.305\times10^{-6}T^2 + 200.075T^{-1} + 202.803\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (207). Entropy and heat capacity at 298 K estimated. High-temperature data based on Dworkin (69).

$GdI_3(g)$

Gadolinium Triiodide (ideal gas)

[Formation: $Gd(c,l) + 1.5I_2(c,l,g) = GdI_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.478	102.176	102.176	0	-75.700	-88.908	65.170
300	19.482	102.296	102.176	.036	-75.716	-88.990	64.829
386.8	19.627	107.268	102.783	1.735	-76.476	-92.737	52.398
386.8	19.627	107.268	102.783	1.735	-82.039	-92.737	52.398
400	19.649	107.927	102.942	1.994	-82.253	-93.099	50.866
458.4	19.695	110.609	103.752	3.143	-83.184	-94.615	45.109
458.4	19.695	110.609	103.752	3.143	-98.215	-94.615	45.109
500	19.728	112.321	104.395	3.963	-98.234	-94.285	41.211
600	19.772	115.922	106.025	5.938	-98.290	-93.479	34.049
700	19.798	118.972	107.662	7.917	-98.366	-92.670	28.932
800	19.815	121.617	109.244	9.898	-98.463	-91.849	25.092
900	19.827	123.952	110.752	11.880	-98.585	-91.016	22.101
1000	19.836	126.041	112.178	13.863	-98.726	-90.174	19.707
1100	19.842	127.932	113.526	15.847	-98.890	-89.301	17.742
1200	19.847	129.659	114.800	17.831	-99.081	-88.430	16.105
1300	19.850	131.248	116.005	19.816	-99.298	-87.534	14.716
1400	19.853	132.719	117.147	21.801	-99.548	-86.609	13.520
1500	19.856	134.089	118.231	23.787	-99.828	-85.675	12.483
1533	19.857	134.521	118.577	24.442	-99.930	-85.364	12.170
1533	19.857	134.521	118.577	24.442	-100.865	-85.364	12.170
1585	19.858	135.183	119.110	25.475	-100.900	-84.843	11.699
1585	19.858	135.183	119.110	25.475	-103.303	-84.843	11.699
1600	19.858	135.370	119.262	25.773	-103.344	-84.670	11.565
1700	19.859	136.574	120.246	27.758	-103.621	-83.494	10.734
1800	19.861	137.709	121.185	29.744	-103.898	-82.298	9.992
1900	19.862	138.783	122.082	31.731	-104.178	-81.089	9.327
2000	19.863	139.802	122.944	33.717	-104.460	-79.878	8.729

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
1533 K, α - β transition point of Gd; $\Delta H°$ = 0.935 kcal/mol.
1585 K, melting point of Gd: $\Delta H°$ = 2.403 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.865 + 0.004\times10^{-3}T - 0.345\times10^{5}T^{-2}$

$H°- H°_{298} = 19.865\times10^{-3}T + 0.002\times10^{-6}T^{2} + 0.345\times10^{2}T^{-1} - 6.039$

GdI_3(g)--continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -76.173 - 2.236\times10^{-3}T - 4.439\times10^{-6}T^2 + 457.600T^{-1}$

$\Delta Gf^\circ = -76.173 + 2.236\times10^{-3}T\ln T + 4.439\times10^{-6}T^2 + 228.800T^{-1} - 59.351\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -78.356 - 11.843\times10^{-3}T - 2.201\times10^{-6}T^2 + 457.600T^{-1}$

$\Delta Gf^\circ = -78.356 + 11.843\times10^{-3}T\ln T + 2.201\times10^{-6}T^2 + 228.800T^{-1} - 110.074\times10^{-3}T$

458.4-1533 K: $\Delta Hf^\circ = -100.426 + 3.668\times10^{-3}T - 2.303\times10^{-6}T^2 + 434.650T^{-1}$

$\Delta Gf^\circ = -100.426 - 3.668\times10^{-3}T\ln T + 2.303\times10^{-6}T^2 + 217.325T^{-1} + 33.120\times10^{-3}T$

1533-1585 K: $\Delta Hf^\circ = -100.067 - 0.373\times10^{-3}T - 0.100\times10^{-6}T^2 + 11.550T^{-1}$

$\Delta Gf^\circ = -100.067 + 0.373\times10^{-3}T\ln T + 0.100\times10^{-6}T^2 + 5.775T^{-1} + 6.713\times10^{-3}T$

1585-2000 K: $\Delta Hf^\circ = -99.216 - 2.426\times10^{-3}T - 0.100\times10^{-6}T^2 + 11.550T^{-1}$

$\Delta Gf^\circ = -99.216 + 2.426\times10^{-3}T\ln T + 0.100\times10^{-6}T^2 + 5.775T^{-1} - 8.951\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

$GeBr_4(g)$

Germanium Tetrabromide (ideal gas)

[Formation: $Ge(c) + 2Br_2(l,g) = GeBr_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	24.340	94.660	94.660	0	-71.700	-76.015	55.720
300	24.360	94.810	94.660	.050	-71.726	-76.036	55.392
332.6	24.543	97.332	94.785	.847	-72.288	-76.476	50.251
332.6	24.543	97.332	94.785	.847	-86.418	-76.476	50.251
400	24.920	101.900	95.625	2.510	-86.325	-74.483	40.695
500	25.260	107.500	97.460	5.020	-86.169	-71.540	31.270
600	25.460	112.130	99.530	7.560	-86.005	-68.624	24.996
700	25.570	116.060	101.617	10.110	-85.848	-65.744	20.526
800	25.600	119.480	103.643	12.670	-85.692	-62.882	17.178
900	25.580	122.490	105.568	15.230	-85.556	-60.034	14.578
1000	25.520	125.180	107.400	17.780	-85.448	-57.214	12.504
1100	25.420	127.610	109.128	20.330	-85.361	-54.392	10.806
1200	25.290	129.820	110.762	22.870	-85.303	-51.576	9.393

Phase change: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp^\circ = 25.880 - 0.176\times10^{-3}T - 1.322\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.880\times10^{-3}T - 0.088\times10^{-6}T^2 + 1.322\times10^{2}T^{-1} - 8.152$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -67.293 - 15.883\times10^{-3}T - 0.354\times10^{-6}T^2 + 107.300T^{-1}$

$\Delta Gf^\circ = -67.293 + 15.883\times10^{-3}T\ln T + 0.354\times10^{-6}T^2 + 53.650T^{-1} - 120.457\times10^{-3}T$

332.6-1200 K: $\Delta Hf^\circ = -87.294 + 2.439\times10^{-3}T - 0.664\times10^{-6}T^2 + 44.500T^{-1}$

$\Delta Gf^\circ = -87.294 - 2.439\times10^{-3}T\ln T + 0.664\times10^{-6}T^2 + 22.250T^{-1} + 46.253\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (252). Other data based on Zaitsev (269).

GeCl(g)

Germanium Monochloride (ideal gas)

[Formation: $Ge(c,l) + 0.5Cl_2(g) = GeCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.839	58.736	58.736	0	17.454	10.101	-7.404
300	8.851	58.790	58.737	.016	17.453	10.055	-7.325
400	9.362	61.413	59.090	.929	17.376	7.599	-4.152
500	9.629	63.535	59.773	1.881	17.311	5.166	-2.258
600	9.731	65.301	60.553	2.849	17.245	2.746	-1.000
700	9.744	66.803	61.340	3.824	17.174	.331	-.103
800	9.714	68.103	62.107	4.797	17.090	-2.070	.565
900	9.669	69.244	62.837	5.766	16.988	-4.455	1.082
1000	9.620	70.260	63.529	6.731	16.864	-6.838	1.494
1100	9.575	71.175	64.184	7.690	16.715	-9.199	1.828
1200	9.536	72.006	64.801	8.646	16.545	-11.545	2.103
1210.4	9.532	72.088	64.863	8.745	16.526	-11.784	2.128
1210.4	9.532	72.088	64.863	8.745	7.696	-11.784	2.128
1300	9.502	72.768	65.385	9.598	7.555	-13.218	2.222
1400	9.475	73.472	65.939	10.546	7.391	-14.810	2.312
1500	9.453	74.124	66.462	11.493	7.225	-16.381	2.387
1600	9.436	74.734	66.961	12.437	7.055	-17.960	2.453
1700	9.424	75.306	67.435	13.380	6.884	-19.518	2.509
1800	9.415	75.844	67.887	14.322	6.710	-21.061	2.557
1900	9.410	76.353	68.320	15.263	6.535	-22.593	2.599
2000	9.408	76.836	68.734	16.204	6.359	-24.119	2.636

Phase change: 1210.4 K, melting point of Ge; ΔH° = 8.830 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 10.321 - 0.532\times10^{-3}T - 1.177\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 10.321\times10^{-3}T - 0.266\times10^{-6}T^2 + 1.177\times10^{2}T^{-1} - 3.448$

Formation equations (kcal/mol):

298.15-1210.4 K: $\Delta Hf^\circ = 17.229 + 0.326\times10^{-3}T - 0.776\times10^{-6}T^2 + 58.650T^{-1}$

$\Delta Gf^\circ = 17.229 - 0.326\times10^{-3}T\ln T + 0.776\times10^{-6}T^2 + 29.325T^{-1} - 22.607\times10^{-3}T$

1210.4-2000 K: $\Delta Hf^\circ = 8.929 - 0.693\times10^{-3}T - 0.310\times10^{-6}T^2 + 83.550T^{-1}$

$\Delta Gf^\circ = 8.929 + 0.693\times10^{-3}T\ln T + 0.310\times10^{-6}T^2 + 41.775T^{-1} - 22.428\times10^{-3}T$

Source: Data from Gurvich (94).

$GeCl_2(g)$

Germanium Dichloride (ideal gas)

[Formation: $Ge(c,l) + Cl_2(g) = GeCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	12.855	70.678	70.678	0	-40.870	-43.839	32.134
300	12.866	70.757	70.678	.024	-40.871	-43.858	31.950
400	13.284	74.523	71.188	1.334	-40.966	-44.841	24.500
500	13.497	77.513	72.165	2.674	-41.069	-45.796	20.017
600	13.619	79.985	73.268	4.030	-41.182	-46.727	17.020
700	13.694	82.091	74.382	5.396	-41.301	-47.647	14.876
800	13.744	83.923	75.463	6.768	-41.429	-48.545	13.262
900	13.778	85.544	76.495	8.144	-41.569	-49.423	12.001
1000	13.803	86.996	77.473	9.523	-41.726	-50.294	10.992
1100	13.821	88.313	78.399	10.905	-41.900	-51.140	10.160
1200	13.835	89.516	79.276	12.288	-42.093	-51.969	9.465
1210.4	13.836	89.635	79.364	12.432	-42.114	-52.050	9.398
1210.4	13.836	89.635	79.364	12.432	-50.944	-52.050	9.398
1300	13.846	90.624	80.107	13.672	-51.102	-52.124	8.763
1400	13.855	91.650	80.895	15.057	-51.281	-52.194	8.148
1500	13.862	92.607	81.645	16.443	-51.461	-52.247	7.612
1600	13.868	93.501	82.358	17.829	-51.643	-52.302	7.144
1700	13.873	94.342	83.038	19.216	-51.825	-52.337	6.728
1800	13.877	95.135	83.688	20.604	-52.008	-52.357	6.357
1900	13.880	95.886	84.312	21.991	-52.193	-52.366	6.023
2000	13.883	96.598	84.908	23.380	-52.379	-52.367	5.722

Phase change: 1210.4 K, melting point of Ge; $\Delta H° = 8.830$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.827 + 0.052\times10^{-3}T - 0.878\times10^{5}T^{-2}$

$H°- H°_{298} = 13.827\times10^{-3}T + 0.026\times10^{-6}T^2 + 0.878\times10^{2}T^{-1} - 4.419$

Formation equations (kcal/mol):

298.15-1210.4 K: $\Delta Hf° = -40.632 - 0.581\times10^{-3}T - 0.528\times10^{-6}T^2 - 5.400T^{-1}$

$\Delta Gf° = -40.632 + 0.581\times10^{-3}T\ln T + 0.528\times10^{-6}T^2 - 2.700T^{-1} - 14.195\times10^{-3}T$

1210.4-2000 K: $\Delta Hf° = -48.932 - 1.600\times10^{-3}T - 0.062\times10^{-6}T^2 + 19.500T^{-1}$

$\Delta Gf° = -48.932 + 1.600\times10^{-3}T\ln T + 0.062\times10^{-6}T^2 + 9.750T^{-1} - 14.015\times10^{-3}T$

Source: Data from Gurvich (94).

$GeCl_3(g)$

Germanium Trichloride (ideal gas)

[Formation: $Ge(c,l) + 1.5Cl_2(g) = GeCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	18.226	80.089	80.089	0	-76.684	-74.515	54.620
300	18.244	80.202	80.089	.034	-76.683	-74.502	54.274
400	18.903	85.552	80.814	1.895	-76.642	-73.783	40.313
500	19.235	89.810	82.202	3.804	-76.602	-73.070	31.939
600	19.423	93.335	83.772	5.738	-76.572	-72.363	26.358
700	19.539	96.338	85.358	7.686	-76.548	-71.668	22.375
800	19.616	98.953	86.898	9.644	-76.533	-70.973	19.389
900	19.669	101.266	88.368	11.608	-76.529	-70.275	17.065
1000	19.707	103.341	89.764	13.577	-76.543	-69.587	15.208
1100	19.735	105.220	91.084	15.550	-76.575	-68.887	13.686
1200	19.757	106.939	92.336	17.524	-76.627	-68.185	12.418
1210.4	19.759	107.109	92.462	17.729	-76.633	-68.108	12.297
1210.4	19.759	107.109	92.462	17.729	-85.463	-68.108	12.297
1300	19.774	108.521	93.520	19.501	-85.494	-66.818	11.233
1400	19.787	109.987	94.645	21.479	-85.532	-65.379	10.206
1500	19.798	111.352	95.713	23.458	-85.572	-63.931	9.315
1600	19.807	112.630	96.731	25.438	-85.614	-62.496	8.537
1700	19.814	113.831	97.702	27.419	-85.657	-61.048	7.848
1800	19.821	114.964	98.630	29.401	-85.701	-59.596	7.236
1900	19.826	116.036	99.519	31.383	-85.747	-58.137	6.687
2000	19.830	117.053	100.370	33.366	-85.797	-56.680	6.194

Phase change: 1210.4 K, melting point of Ge; ΔH° = 8.830 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.770 + 0.062\times10^{-3}T - 1.389\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.770\times10^{-3}T + 0.031\times10^{-6}T^2 + 1.389\times10^{2}T^{-1} - 6.363$

Formation equations (kcal/mol):

298.15-1210.4 K: $\Delta Hf^\circ = -76.955 + 0.948\times10^{-3}T - 0.567\times10^{-6}T^2 + 11.550T^{-1}$

$\Delta Gf^\circ = -76.955 - 0.948\times10^{-3}T\ln T + 0.567\times10^{-6}T^2 + 5.775T^{-1} + 13.356\times10^{-3}T$

1210.4-2000 K: $\Delta Hf^\circ = -85.255 - 0.070\times10^{-3}T - 0.101\times10^{-6}T^2 + 36.450T^{-1}$

$\Delta Gf^\circ = -85.255 + 0.070\times10^{-3}T\ln T + 0.101\times10^{-6}T^2 + 18.225T^{-1} + 13.535\times10^{-3}T$

Source: Data from Gurvich (94).

$GeCl_4(g)$

Germanium Tetrachloride (ideal gas)

[Formation: $Ge(c,l) + 2Cl_2(g) = GeCl_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	22.925	83.241	83.241	0	-119.500	-110.326	80.870
300	22.954	83.383	83.241	.043	-119.497	-110.270	80.331
400	24.080	90.160	84.158	2.401	-119.374	-107.214	58.578
500	24.667	95.602	85.920	4.841	-119.230	-104.187	45.540
600	25.006	100.132	87.922	7.326	-119.083	-101.189	36.857
700	25.217	104.004	89.950	9.838	-118.934	-98.222	30.666
800	25.358	107.381	91.922	12.367	-118.791	-95.275	26.028
900	25.455	110.374	93.810	14.908	-118.656	-92.340	22.423
1000	25.526	113.059	95.602	17.457	-118.537	-89.430	19.545
1100	25.578	115.495	97.302	20.012	-118.435	-86.523	17.190
1200	25.619	117.722	98.912	22.572	-118.351	-83.623	15.230
1210.4	25.622	117.943	99.075	22.838	-118.343	-83.318	15.044
1210.4	25.622	117.943	99.075	22.838	-127.173	-83.318	15.044
1300	25.650	119.774	100.439	25.136	-127.082	-80.071	13.461
1400	25.675	121.676	101.889	27.702	-126.984	-76.458	11.935
1500	25.695	123.448	103.267	30.271	-126.887	-72.845	10.613
1600	25.712	125.107	104.581	32.841	-126.793	-69.255	9.460
1700	25.726	126.666	105.835	35.413	-126.699	-65.659	8.441
1800	25.737	128.137	107.034	37.986	-126.608	-62.069	7.536
1900	25.747	129.529	108.181	40.561	-126.517	-58.476	6.726
2000	25.756	130.850	109.282	43.136	-126.432	-54.896	5.999

Phase changes: 356 K, boiling point of $GeCl_4$; $\Delta H°$ = 8.1 kcal/mol.
1210.4 K, melting point of Ge; $\Delta H°$ = 8.830 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 25.524 + 0.198\times10^{-3}T - 2.363\times10^{5}T^{-2}$

$H°- H°_{298} = 25.524\times10^{-3}T + 0.099\times10^{-6}T^{2} + 2.363\times10^{2}T^{-1} - 8.411$

Formation equations (kcal/mol):

298.15-1210.4 K: $\Delta Hf° = -120.385 + 2.289\times10^{-3}T - 0.543\times10^{-6}T^{2} + 74.800T^{-1}$

$\Delta Gf° = -120.385 - 2.289\times10^{-3}T\ln T + 0.543\times10^{-6}T^{2} + 37.400T^{-1} + 46.197\times10^{-3}T$

1210.4-2000 K: $\Delta Hf° = -128.685 + 1.270\times10^{-3}T - 0.077\times10^{-6}T^{2} + 99.700T^{-1}$

$\Delta Gf° = -128.685 - 1.270\times10^{-3}T\ln T + 0.077\times10^{-6}T^{2} + 49.850T^{-1} + 46.376\times10^{-3}T$

Sources: Vaporization data from Golubenko (90). Other data from Gurvich (94).

GeF(g)

Germanium Monofluoride (ideal gas)

[Formation: $Ge(c,l) + 0.5F_2(g) = GeF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.313	55.903	55.903	0	-15.918	-23.149	16.968
300	8.328	55.954	55.904	.015	-15.920	-23.195	16.897
400	8.978	58.446	56.238	.883	-16.011	-25.606	13.990
500	9.333	60.493	56.891	1.801	-16.086	-27.994	12.236
600	9.491	62.211	57.639	2.743	-16.159	-30.366	11.061
700	9.541	63.678	58.398	3.696	-16.236	-32.730	10.219
800	9.538	64.952	59.140	4.650	-16.328	-35.080	9.583
900	9.513	66.075	59.849	5.603	-16.436	-37.415	9.086
1000	9.481	67.076	60.524	6.552	-16.569	-39.747	8.687
1100	9.448	67.978	61.161	7.499	-16.724	-42.055	8.355
1200	9.419	68.798	61.763	8.442	-16.903	-44.347	8.077
1210.4	9.416	68.879	61.824	8.540	-16.922	-44.581	8.049
1210.4	9.416	68.879	61.824	8.540	-25.752	-44.581	8.049
1300	9.393	69.551	62.333	9.383	-25.900	-45.966	7.727
1400	9.371	70.246	62.874	10.321	-26.072	-47.502	7.415
1500	9.353	70.892	63.387	11.257	-26.248	-49.020	7.142
1600	9.340	71.495	63.876	12.191	-26.427	-50.542	6.904
1700	9.329	72.061	64.340	13.125	-26.607	-52.043	6.690
1800	9.322	72.594	64.784	14.058	-26.790	-53.529	6.499
1900	9.317	73.098	65.209	14.990	-26.974	-55.003	6.327
2000	9.314	73.576	65.615	15.921	-27.162	-56.471	6.171

Phase change: 1210.4 K, melting point of Ge; ΔH° = 8.830 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 10.104 - 0.442\times10^{-3}T - 1.475\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 10.104\times10^{-3}T - 0.221\times10^{-6}T^2 + 1.475\times10^{2}T^{-1} - 3.488$

Formation equations (kcal/mol):

298.15-1210.4 K: $\Delta Hf^\circ = -16.172 + 0.269\times10^{-3}T - 0.774\times10^{-6}T^2 + 72.350T^{-1}$

$\Delta Gf^\circ = -16.172 - 0.269\times10^{-3}T\ln T + 0.774\times10^{-6}T^2 + 36.175T^{-1} - 22.504\times10^{-3}T$

1210.4-2000 K: $\Delta Hf^\circ = -24.472 - 0.750\times10^{-3}T - 0.308\times10^{-6}T^2 + 97.250T^{-1}$

$\Delta Gf^\circ = -24.472 + 0.750\times10^{-3}T\ln T + 0.308\times10^{-6}T^2 + 48.625T^{-1} - 22.325\times10^{-3}T$

Source: Data from Gurvich (94).

$GeF_2(g)$

Germanium Difluoride (ideal gas)

[Formation: $Ge(c,l) + F_2(g) = GeF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	11.436	64.692	64.692	0	-137.190	-139.819	102.489
300	11.455	64.762	64.692	.021	-137.193	-139.837	101.870
400	12.272	68.180	65.153	1.211	-137.347	-140.695	76.871
500	12.767	70.976	66.046	2.465	-137.487	-141.513	61.855
600	13.076	73.333	67.070	3.758	-137.624	-142.303	51.833
700	13.278	75.365	68.114	5.076	-137.761	-143.076	44.670
800	13.416	77.147	69.132	6.412	-137.901	-143.825	39.291
900	13.514	78.733	70.113	7.758	-138.052	-144.554	35.102
1000	13.586	80.161	71.047	9.114	-138.218	-145.274	31.749
1100	13.641	81.459	71.936	10.475	-138.402	-145.969	29.001
1200	13.682	82.647	72.780	11.841	-138.603	-146.645	26.707
1210.4	13.685	82.765	72.865	11.983	-138.625	-146.711	26.490
1210.4	13.685	82.765	72.865	11.983	-147.455	-146.711	26.490
1300	13.715	83.744	73.582	13.211	-147.619	-146.647	24.653
1400	13.741	84.762	74.345	14.584	-147.806	-146.566	22.880
1500	13.763	85.710	75.071	15.959	-147.994	-146.462	21.339
1600	13.780	86.599	75.763	17.337	-148.182	-146.363	19.992
1700	13.795	87.435	76.426	18.715	-148.372	-146.244	18.801
1800	13.807	88.224	77.060	20.096	-148.563	-146.108	17.740
1900	13.818	88.971	77.667	21.477	-148.755	-145.960	16.789
2000	13.827	89.680	78.251	22.859	-148.950	-145.806	15.933

Phase change: 1210.4 K, melting point of Ge; $\Delta H° = 8.830$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.412 + 0.290\times10^{-3}T - 1.834\times10^{5}T^{-2}$

$H°- H°_{298} = 13.412\times10^{-3}T + 0.145\times10^{-6}T^{2} + 1.834\times10^{2}T^{-1} - 4.627$

Formation equations (kcal/mol):

298.15-1210.4 K: $\Delta Hf° = -137.139 - 0.677\times10^{-3}T - 0.495\times10^{-6}T^{2} + 58.000T^{-1}$

$\Delta Gf° = -137.139 + 0.677\times10^{-3}T\ln T + 0.495\times10^{-6}T^{2} + 29.000T^{-1} - 13.322\times10^{-3}T$

1210.4-2000 K: $\Delta Hf° = -145.439 - 1.696\times10^{-3}T - 0.029\times10^{-6}T^{2} + 82.900T^{-1}$

$\Delta Gf° = -145.439 + 1.696\times10^{-3}T\ln T + 0.029\times10^{-6}T^{2} + 41.450T^{-1} - 13.143\times10^{-3}T$

Source: Data from Gurvich (94).

$GeF_3(g)$

Germanium Trifluoride (ideal gas)

[Formation: $Ge(c,l) + 1.5F_2(g) = GeF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	15.817	71.130	71.130	0	-179.970	-177.297	129.961
300	15.850	71.228	71.131	.029	-179.972	-177.282	129.148
400	17.213	75.991	71.771	1.688	-180.042	-176.374	96.365
500	18.024	79.927	72.977	3.475	-180.050	-175.429	76.679
600	18.527	83.261	74.456	5.283	-180.087	-174.522	63.569
700	18.854	86.143	75.924	7.153	-180.096	-173.597	54.199
800	19.077	88.676	77.364	9.050	-180.106	-172.669	47.170
900	19.236	90.933	78.747	10.967	-180.122	-171.734	41.702
1000	19.352	92.966	80.070	12.896	-180.155	-170.808	37.330
1100	19.439	94.815	81.328	14.836	-180.203	-169.869	33.749
1200	19.506	96.509	82.523	16.783	-180.268	-168.924	30.765
1210.4	19.512	96.677	82.644	16.986	-180.276	-168.822	30.482
1210.4	19.512	96.677	82.644	16.986	-189.106	-168.822	30.482
1300	19.559	98.072	83.659	18.737	-189.148	-167.313	28.128
1400	19.601	99.523	84.741	20.695	-189.200	-165.632	25.856
1500	19.635	100.877	85.772	22.657	-189.253	-163.941	23.886
1600	19.663	102.145	86.757	24.621	-189.307	-162.261	22.164
1700	19.687	103.338	87.697	26.589	-189.361	-160.568	20.642
1800	19.707	104.464	88.598	28.559	-189.419	-158.868	19.289
1900	19.723	105.530	89.462	30.530	-189.478	-157.163	18.078
2000	19.738	106.542	90.291	32.503	-189.541	-155.458	16.987

Phase change: 1210.4 K, melting point of Ge; ΔH° = 8.830 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.019 + 0.528\times10^{-3}T - 2.986\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.019\times10^{-3}T + 0.264\times10^{-6}T^2 + 2.986\times10^{2}T^{-1} - 6.695$

Formation equations (kcal/mol):

298.15-1210.4 K: $\Delta Hf^\circ = -180.543 + 0.676\times10^{-3}T - 0.463\times10^{-6}T^2 + 122.950T^{-1}$

$\Delta Gf^\circ = -180.543 - 0.676\times10^{-3}T\ln T + 0.463\times10^{-6}T^2 + 61.475T^{-1} + 13.908\times10^{-3}T$

1210.4-2000 K: $\Delta Hf^\circ = -188.843 - 0.343\times10^{-3}T + 0.003\times10^{-6}T^2 + 147.850T^{-1}$

$\Delta Gf^\circ = -188.843 + 0.343\times10^{-3}T\ln T - 0.003\times10^{-6}T^2 + 73.925T^{-1} + 14.087\times10^{-3}T$

Source: Data from Gurvich (94).

$GeF_4(g)$

Germanium Tetrafluoride (ideal gas)

[Formation: $Ge(c,l) + 2F_2(g) = GeF_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	19.503	72.130	72.130	0	-284.450	-274.854	201.471
300	19.548	72.256	72.130	.039	-284.449	-274.794	200.185
400	21.518	78.171	72.921	2.100	-284.501	-271.565	148.375
500	22.765	83.117	74.479	4.319	-284.480	-268.331	117.286
600	23.568	87.344	76.281	6.638	-284.421	-265.103	96.563
700	24.104	91.020	78.129	9.024	-284.338	-261.893	81.766
800	24.475	94.264	79.947	11.454	-284.246	-258.694	70.671
900	24.741	97.163	81.702	13.915	-284.153	-255.502	62.043
1000	24.937	99.780	83.380	16.400	-284.070	-252.330	55.146
1100	25.086	102.164	84.981	18.901	-284.000	-249.156	49.502
1200	25.200	104.352	86.505	21.416	-283.943	-245.989	44.800
1210.4	25.209	104.569	86.660	21.678	-283.938	-245.656	44.355
1210.4	25.209	104.569	86.660	21.678	-292.768	-245.656	44.355
1300	25.291	106.373	87.958	23.940	-292.700	-242.168	40.712
1400	25.364	108.250	89.341	26.473	-292.627	-238.285	37.197
1500	25.423	110.002	90.661	29.012	-292.554	-234.399	34.151
1600	25.471	111.644	91.921	31.557	-292.481	-230.532	31.489
1700	25.512	113.190	93.127	34.107	-292.407	-226.661	29.139
1800	25.546	114.649	94.283	36.659	-292.339	-222.792	27.050
1900	25.575	116.031	95.391	39.216	-292.268	-218.922	25.181
2000	25.600	117.343	96.456	41.774	-292.204	-215.062	23.501

Phase change: 1210.4 K, melting point of Ge; $\Delta H° = 8.830$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 24.170 + 0.992\times10^{-3}T - 4.412\times10^{5}T^{-2}$

$H°-H°_{298} = 24.170\times10^{-3}T + 0.496\times10^{-6}T^2 + 4.412\times10^{2}T^{-1} - 8.730$

Formation equations (kcal/mol):

298.15-1210.4 K: $\Delta Hf° = -285.613 + 1.573\times10^{-3}T - 0.318\times10^{-6}T^2 + 215.300T^{-1}$

$\Delta Gf° = -285.613 - 1.573\times10^{-3}T\ln T + 0.318\times10^{-6}T^2 + 107.650T^{-1} + 43.743\times10^{-3}T$

1210.4-2000 K: $\Delta Hf° = -293.913 + 0.554\times10^{-3}T + 0.148\times10^{-6}T^2 + 240.200T^{-1}$

$\Delta Gf° = -293.913 - 0.554\times10^{-3}T\ln T - 0.148\times10^{-6}T^2 + 120.100T^{-1} + 43.922\times10^{-3}T$

Source: Data from Gurvich (94).

GeI_4(g)

Germanium Tetraiodide (ideal gas)

[Formation: $Ge(c) + 2I_2(c,l,g) = GeI_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	24.890	102.490	102.490	0	-13.600	-25.390	18.611
300	24.900	102.640	102.490	.050	-13.608	-25.459	18.546
386.8	25.212	109.013	103.256	2.227	-14.345	-28.799	16.272
386.8	25.212	109.013	103.256	2.227	-21.763	-28.799	16.272
400	25.260	109.860	103.460	2.560	-22.017	-29.035	15.864
458.4	25.388	113.311	104.515	4.032	-23.138	-29.983	14.295
458.4	25.388	113.311	104.515	4.032	-43.180	-29.983	14.295
500	25.480	115.520	105.340	5.090	-43.113	-28.785	12.582
600	25.610	120.180	107.430	7.650	-42.947	-25.929	9.444
700	25.670	124.140	109.554	10.210	-42.792	-23.118	7.218
800	25.690	127.560	111.585	12.780	-42.638	-20.307	5.547
900	25.670	130.590	113.534	15.350	-42.502	-17.525	4.256
1000	25.630	133.290	115.370	17.920	-42.384	-14.754	3.224
1100	25.560	135.730	117.112	20.480	-42.297	-11.994	2.383
1200	25.480	137.950	118.758	23.030	-42.241	-9.241	1.683

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp^\circ = 26.009 - 0.288\times10^{-3}T - 0.919\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 26.009\times10^{-3}T - 0.144\times10^{-6}T^2 + 0.919\times10^{2}T^{-1} - 8.050$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -11.917 - 5.326\times10^{-3}T - 3.594\times10^{-6}T^2 + 67.000T^{-1}$

$\Delta Gf^\circ = -11.917 + 5.326\times10^{-3}T\ln T + 3.594\times10^{-6}T^2 + 33.500T^{-1} - 76.982\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -14.828 - 18.134\times10^{-3}T - 0.610\times10^{-6}T^2 + 67.000T^{-1}$

$\Delta Gf^\circ = -14.828 + 18.134\times10^{-3}T\ln T + 0.610\times10^{-6}T^2 + 33.500T^{-1} - 144.612\times10^{-3}T$

458.4-1200 K: $\Delta Hf^\circ = -44.254 + 2.546\times10^{-3}T - 0.746\times10^{-6}T^2 + 36.400T^{-1}$

$\Delta Gf^\circ = -44.254 - 2.546\times10^{-3}T\ln T + 0.746\times10^{-6}T^2 + 18.200T^{-1} + 46.314\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (252). Other data based on Zaitsev (269).

HBr(g)

Hydrogen Bromide (ideal gas)

[Formation: $0.5H_2(g) + 0.5Br_2(l,g) = HBr(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	6.965	47.463	47.463	0	-8.695	-12.771	9.361
300	6.965	47.506	47.463	.013	-8.705	-12.796	9.322
332.6	6.971	48.225	47.503	.240	-8.884	-13.231	8.694
332.6	6.971	48.225	47.503	.240	-12.417	-13.231	8.694
400	6.984	49.512	47.737	.710	-12.476	-13.392	7.317
500	7.040	51.076	48.254	1.411	-12.566	-13.611	5.949
600	7.139	52.367	48.834	2.120	-12.651	-13.811	5.031
700	7.272	53.477	49.420	2.840	-12.728	-13.998	4.370
800	7.423	54.458	49.989	3.575	-12.793	-14.175	3.872
900	7.576	55.341	50.535	4.325	-12.849	-14.344	3.483
1000	7.725	56.147	51.057	5.090	-12.892	-14.508	3.171
1100	7.863	56.890	51.555	5.869	-12.928	-14.669	2.914
1200	7.989	57.580	52.028	6.662	-12.954	-14.825	2.700
1300	8.103	58.224	52.481	7.466	-12.976	-14.981	2.519
1400	8.205	58.828	52.912	8.282	-12.990	-15.134	2.362
1500	8.296	59.397	53.326	9.107	-13.003	-15.287	2.227
1600	8.378	59.935	53.722	9.941	-13.012	-15.438	2.109
1700	8.451	60.446	54.104	10.782	-13.020	-15.592	2.004
1800	8.517	60.931	54.469	11.631	-13.024	-15.742	1.911
1900	8.577	61.393	54.821	12.486	-13.028	-15.892	1.828
2000	8.630	61.834	55.161	13.346	-13.033	-16.043	1.753
2100	8.679	62.256	55.488	14.212	-13.035	-16.192	1.685
2200	8.724	62.661	55.806	15.082	-13.040	-16.344	1.624
2300	8.765	63.050	56.113	15.956	-13.043	-16.495	1.567
2400	8.803	63.424	56.409	16.835	-13.047	-16.643	1.516
2500	8.838	63.784	56.697	17.717	-13.051	-16.793	1.468
2600	8.870	64.131	56.976	18.602	-13.056	-16.942	1.424
2700	8.900	64.466	57.247	19.491	-13.060	-17.091	1.383
2800	8.929	64.790	57.511	20.382	-13.067	-17.240	1.346
2900	8.955	65.104	57.767	21.276	-13.074	-17.390	1.311
3000	8.980	65.408	58.017	22.173	-13.080	-17.538	1.278

Phase change: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 6.474 + 1.172\times10^{-3}T + 0.126\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 6.474\times10^{-3}T + 0.586\times10^{-6}T^2 - 0.126\times10^{2}T^{-1} - 1.940$

2000-3000 K: $Cp^\circ = 8.825 + 0.112\times10^{-3}T - 16.800\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.825\times10^{-3}T + 0.056\times10^{-6}T^2 + 16.800\times10^{2}T^{-1} - 5.368$

HBr(g) - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -6.989 - 5.799\times10^{-3}T + 0.427\times10^{-6}T^2 - 4.350T^{-1}$

$\Delta Gf^\circ = -6.989 + 5.799\times10^{-3}T\ln T - 0.427\times10^{-6}T^2 - 2.175T^{-1} - 52.283\times10^{-3}T$

332.6-2000 K: $\Delta Hf^\circ = -11.989 - 1.219\times10^{-3}T + 0.349\times10^{-6}T^2 - 20.050T^{-1}$

$\Delta Gf^\circ = -11.989 + 1.219\times10^{-3}T\ln T - 0.349\times10^{-6}T^2 - 10.025T^{-1} - 10.605\times10^{-3}T$

2000-3000 K: $\Delta Hf^\circ = -15.418 + 1.132\times10^{-3}T - 0.181\times10^{-6}T^2 + 1672.550T^{-1}$

$\Delta Gf^\circ = -15.418 - 1.132\times10^{-3}T\ln T + 0.181\times10^{-6}T^2 + 836.275T^{-1} + 7.707\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from CODATA (34). Other data from JANAF (60).

HCl(g)

Hydrogen Chloride (ideal gas)

[Formation: $0.5H_2(g) + 0.5Cl_2(g) = HCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	6.964	44.643	44.643	0	-22.063	-22.777	16.696
300	6.964	44.686	44.643	.013	-22.064	-22.781	16.596
400	6.973	46.691	44.916	.710	-22.129	-23.011	12.572
500	7.004	48.250	45.434	1.408	-22.207	-23.223	10.151
600	7.069	49.532	46.012	2.112	-22.288	-23.418	8.530
700	7.167	50.628	46.595	2.823	-22.367	-23.601	7.368
800	7.289	51.593	47.160	3.546	-22.440	-23.772	6.494
900	7.423	52.459	47.702	4.281	-22.505	-23.935	5.812
1000	7.559	53.248	48.218	5.030	-22.562	-24.091	5.265
1100	7.693	53.975	48.709	5.793	-22.611	-24.241	4.816
1200	7.819	54.650	49.176	6.569	-22.653	-24.387	4.441
1300	7.936	55.281	49.623	7.356	-22.690	-24.532	4.124
1400	8.043	55.873	50.048	8.155	-22.721	-24.672	3.851
1500	8.141	56.431	50.454	8.965	-22.747	-24.809	3.615
1600	8.229	56.959	50.845	9.783	-22.771	-24.947	3.408
1700	8.310	57.461	51.220	10.610	-22.793	-25.082	3.224
1800	8.382	57.938	51.580	11.445	-22.812	-25.216	3.062
1900	8.449	58.393	51.926	12.287	-22.829	-25.348	2.916
2000	8.509	58.828	52.260	13.135	-22.846	-25.480	2.784
2100	8.564	59.244	52.583	13.988	-22.861	-25.611	2.665
2200	8.614	59.644	52.895	14.847	-22.878	-25.744	2.557
2300	8.660	60.028	53.197	15.711	-22.892	-25.873	2.458
2400	8.703	60.397	53.489	16.579	-22.908	-26.000	2.368
2500	8.742	60.753	53.773	17.451	-22.924	-26.129	2.284
2600	8.778	61.097	54.048	18.327	-22.941	-26.259	2.207
2700	8.812	61.429	54.315	19.207	-22.958	-26.386	2.136
2800	8.844	61.750	54.575	20.090	-22.977	-26.512	2.069
2900	8.874	62.061	54.828	20.976	-22.997	-26.639	2.008
3000	8.902	62.362	55.074	21.864	-23.018	-26.763	1.950

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 6.386 + 1.128\times10^{-3}T + 0.215\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 6.386\times10^{-3}T + 0.564\times10^{-6}T^2 - 0.215\times10^{2}T^{-1} - 1.882$

2000-3000 K: $Cp^\circ = 8.185 + 0.286\times10^{-3}T - 9.882\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.185\times10^{-3}T + 0.143\times10^{-6}T^2 + 9.882\times10^{2}T^{-1} - 4.301$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -21.557 - 1.255\times10^{-3}T + 0.311\times10^{-6}T^2 - 47.400T^{-1}$

$\Delta Gf^\circ = -21.557 + 1.255\times10^{-3}T\ln T - 0.311\times10^{-6}T^2 - 23.700T^{-1} - 10.885\times10^{-3}T$

2000-3000 K: $\Delta Hf^\circ = -23.976 + 0.544\times10^{-3}T - 0.111\times10^{-6}T^2 + 962.300T^{-1}$

$\Delta Gf^\circ = -23.976 - 0.544\times10^{-3}T\ln T + 0.111\times10^{-6}T^2 + 481.150T^{-1} + 3.030\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from CODATA (34). Other data from JANAF (60).

DCl(g)

Deuterium Chloride (ideal gas)

[Formation: $0.5D_2(g) + 0.5Cl_2(g) = DCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	6.972	46.040	46.040	0	-22.310	-22.932	16.809
300	6.972	46.083	46.040	.013	-22.311	-22.935	16.708
400	7.028	48.095	46.315	.712	-22.376	-23.135	12.640
500	7.149	49.675	46.833	1.421	-22.444	-23.315	10.191
600	7.316	50.993	47.420	2.144	-22.507	-23.484	8.554
700	7.501	52.135	48.014	2.885	-22.561	-23.642	7.381
800	7.682	53.148	48.593	3.644	-22.607	-23.793	6.500
900	7.850	54.063	49.152	4.420	-22.644	-23.940	5.813
1000	7.999	54.898	49.685	5.213	-22.673	-24.083	5.263
1100	8.130	55.666	50.193	6.020	-22.695	-24.222	4.812
1200	8.244	56.379	50.681	6.838	-22.715	-24.361	4.437
1300	8.343	57.043	51.145	7.668	-22.732	-24.497	4.118
1400	8.429	57.664	51.588	8.507	-22.745	-24.632	3.845
1500	8.504	58.248	52.013	9.353	-22.759	-24.766	3.608
1600	8.570	58.799	52.420	10.207	-22.770	-24.899	3.401
1700	8.628	59.320	52.810	11.067	-22.780	-25.031	3.218
1800	8.680	59.815	53.186	11.932	-22.791	-25.164	3.055
1900	8.727	60.286	53.548	12.803	-22.800	-25.295	2.910
2000	8.768	60.734	53.895	13.678	-22.811	-25.425	2.778

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 6.515 + 1.354\times10^{-3}T + 0.047\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 6.515\times10^{-3}T + 0.677\times10^{-6}T^2 - 0.047\times10^{2}T^{-1} - 1.987$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -21.951 - 1.031\times10^{-3}T + 0.319\times10^{-6}T^2 - 23.800T^{-1}$

$\Delta Gf^\circ = -21.951 + 1.031\times10^{-3}T\ln T - 0.319\times10^{-6}T^2 - 11.900T^{-1} - 8.931\times10^{-3}T$

Source: Data from Chase (24).

HF(g)

Hydrogen Fluoride (ideal gas)

[Formation: $0.5H_2(g) + 0.5F_2(g) = HF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	6.964	41.508	41.508	0	-65.320	-65.822	48.248
300	6.964	41.551	41.508	.013	-65.320	-65.825	47.953
400	6.967	43.555	41.783	.709	-65.356	-65.989	36.054
500	6.972	45.110	42.298	1.406	-65.410	-66.141	28.910
600	6.986	46.383	42.876	2.104	-65.478	-66.281	24.143
700	7.015	47.461	43.455	2.804	-65.552	-66.409	20.733
800	7.063	48.401	44.016	3.508	-65.632	-66.526	18.174
900	7.129	49.237	44.551	4.217	-65.715	-66.633	16.180
1000	7.211	49.992	45.058	4.934	-65.797	-66.731	14.584
1100	7.303	50.683	45.538	5.660	-65.877	-66.819	13.276
1200	7.402	51.323	45.994	6.395	-65.955	-66.902	12.184
1300	7.504	51.920	46.428	7.140	-66.031	-66.978	11.260
1400	7.606	52.479	46.839	7.896	-66.103	-67.047	10.466
1500	7.705	53.007	47.233	8.661	-66.173	-67.113	9.778
1600	7.800	53.508	47.610	9.437	-66.238	-67.174	9.175
1700	7.891	53.983	47.971	10.221	-66.301	-67.229	8.643
1800	7.977	54.437	48.318	11.015	-66.362	-67.283	8.169
1900	8.058	54.870	48.651	11.816	-66.421	-67.332	7.745
2000	8.133	55.286	48.973	12.626	-66.477	-67.379	7.363
2100	8.204	55.684	49.283	13.443	-66.530	-67.421	7.017
2200	8.270	56.067	49.582	14.267	-66.582	-67.463	6.702
2300	8.331	56.436	49.872	15.097	-66.633	-67.502	6.414
2400	8.389	56.792	50.153	15.933	-66.682	-67.539	6.150
2500	8.442	57.136	50.426	16.774	-66.731	-67.576	5.907
2600	8.493	57.468	50.691	17.621	-66.778	-67.608	5.683
2700	8.540	57.789	50.947	18.473	-66.824	-67.638	5.475
2800	8.584	58.101	51.198	19.329	-66.870	-67.669	5.282
2900	8.625	58.403	51.441	20.189	-66.916	-67.697	5.102
3000	8.664	58.696	51.678	21.054	-66.960	-67.722	4.933

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 6.354 + 0.882\times10^{-3}T + 0.306\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 6.354\times10^{-3}T + 0.441\times10^{-6}T^2 - 0.306\times10^{2}T^{-1} - 1.831$

2000-3000 K: $Cp^\circ = 8.225 + 0.226\times10^{-3}T - 21.738\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.225\times10^{-3}T + 0.113\times10^{-6}T^2 + 21.738\times10^{2}T^{-1} - 5.363$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -64.753 - 1.128\times10^{-3}T + 0.144\times10^{-6}T^2 - 72.600T^{-1}$

$\Delta Gf^\circ = -64.753 + 1.128\times10^{-3}T\ln T - 0.144\times10^{-6}T^2 - 36.300T^{-1} - 9.560\times10^{-3}T$

2000-3000 K: $\Delta Hf^\circ = -68.285 + 0.743\times10^{-3}T - 0.184\times10^{-6}T^2 + 2131.800T^{-1}$

$\Delta Gf^\circ = -68.285 - 0.743\times10^{-3}T\ln T + 0.184\times10^{-6}T^2 + 1065.900T^{-1} + 5.496\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from CODATA (34). Other data from Chase (24).

DF(g)

Deuterium Fluoride (ideal gas)

[Formation: $0.5D_2(g) + 0.5F_2(g) = DF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	6.964	42.924	42.924	0	-65.850	-66.265	48.573
300	6.964	42.967	42.924	.013	-65.850	-66.268	48.275
400	6.973	44.971	43.196	.710	-65.887	-66.401	36.279
500	7.002	46.530	43.714	1.408	-65.941	-66.524	29.077
600	7.065	47.811	44.293	2.111	-66.006	-66.635	24.271
700	7.161	48.907	44.876	2.822	-66.075	-66.735	20.835
800	7.281	49.871	45.441	3.544	-66.145	-66.824	18.255
900	7.413	50.736	45.982	4.279	-66.214	-66.904	16.246
1000	7.549	51.524	46.497	5.027	-66.280	-66.978	14.638
1100	7.681	52.250	46.988	5.788	-66.343	-67.045	13.321
1200	7.806	52.924	47.455	6.563	-66.402	-67.106	12.221
1300	7.923	53.553	47.900	7.349	-66.458	-67.162	11.291
1400	8.029	54.144	48.325	8.147	-66.511	-67.214	10.493
1500	8.126	54.702	48.732	8.955	-66.561	-67.264	9.800
1600	8.215	55.229	49.122	9.772	-66.608	-67.308	9.194
1700	8.295	55.730	49.496	10.598	-66.652	-67.351	8.658
1800	8.367	56.206	49.855	11.431	-66.696	-67.390	8.182
1900	8.433	56.660	50.202	12.271	-66.736	-67.427	7.756
2000	8.493	57.094	50.536	13.117	-66.777	-67.463	7.372

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 6.255 + 1.240\times10^{-3}T + 0.302\times10^{5}T^{-2}$

$H°- H°_{298} = 6.255\times10^{-3}T + 0.620\times10^{-6}T^{2} - 0.302\times10^{2}T^{-1} - 1.819$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -65.313 - 1.131\times10^{-3}T + 0.218\times10^{-6}T^{2} - 65.400T^{-1}$

$\Delta Gf° = -65.313 + 1.131\times10^{-3}T\ln T - 0.218\times10^{-6}T^{2} - 32.700T^{-1} - 9.205\times10^{-3}T$

Source: Data from Chase (24).

$(HF)_2(g)$

Dimeric Hydrogen Fluoride (ideal gas)

[Formation: $H_2(g) + F_2(g) = (HF)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	10.725	57.060	57.060	0	-136.870	-130.135	95.390
300	10.748	57.127	57.060	.020	-136.877	-130.093	94.772
400	11.879	60.378	57.495	1.153	-137.207	-127.779	69.815
500	12.795	63.131	58.355	2.388	-137.475	-125.391	54.808
600	13.512	65.530	59.355	3.705	-137.688	-122.954	44.785
700	14.090	67.658	60.392	5.086	-137.857	-120.484	37.616
800	14.579	69.572	61.422	6.520	-137.991	-117.993	32.234
900	15.012	71.315	62.426	8.000	-138.093	-115.487	28.044
1000	15.404	72.917	63.396	9.521	-138.170	-112.972	24.690
1100	15.763	74.402	64.329	11.080	-138.223	-110.448	21.944
1200	16.093	75.788	65.227	12.673	-138.257	-107.921	19.655
1300	16.396	77.088	66.090	14.298	-138.273	-105.391	17.718
1400	16.673	78.314	66.920	15.951	-138.276	-102.864	16.058
1500	16.926	79.473	67.719	17.631	-138.266	-100.336	14.619
1600	17.155	80.573	68.488	19.336	-138.244	-97.807	13.360
1700	17.364	81.619	69.230	21.062	-138.213	-95.278	12.249
1800	17.553	82.617	69.946	22.808	-138.176	-92.755	11.262
1900	17.724	83.571	70.638	24.572	-138.131	-90.232	10.379
2000	17.880	84.484	71.308	26.352	-138.083	-87.713	9.585

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.057 + 3.352\times10^{-3}T - 2.072\times10^{5}T^{-2}$

$H°- H°_{298} = 12.057\times10^{-3}T + 1.676\times10^{-6}T^{2} + 2.072\times10^{2}T^{-1} - 4.439$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -136.513 - 2.907\times10^{-3}T + 1.083\times10^{-6}T^{2} + 123.200T^{-1}$

$\Delta Gf° = -136.513 + 2.907\times10^{-3}T\ln T - 1.083\times10^{-6}T^{2} + 61.600T^{-1} + 4.459\times10^{-3}T$

Source: Data from Chase (24).

$(HF)_3(g)$

Trimeric Hydrogen Fluoride (ideal gas)

[Formation: $1.5H_2(g) + 1.5F_2(g) = (HF)_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.128	68.917	68.917	0	-210.110	-195.036	142.964
300	18.177	69.029	68.917	.034	-210.117	-194.943	142.014
400	20.394	74.582	69.660	1.969	-210.376	-189.841	103.723
500	21.931	79.308	71.128	4.090	-210.510	-184.689	80.727
600	23.063	83.411	72.841	6.342	-210.553	-179.521	65.390
700	23.973	87.036	74.615	8.695	-210.525	-174.350	54.434
800	24.755	90.290	76.375	11.132	-210.439	-169.189	46.220
900	25.449	93.246	78.087	13.643	-210.301	-164.038	39.833
1000	26.071	95.960	79.740	16.220	-210.122	-158.909	34.729
1100	26.629	98.472	81.331	18.855	-209.905	-153.798	30.556
1200	27.128	100.810	82.857	21.543	-209.657	-148.707	27.083
1300	27.571	103.000	84.324	24.279	-209.383	-143.638	24.147
1400	27.966	105.058	85.732	27.056	-209.090	-138.594	21.635
1500	28.315	106.999	87.086	29.870	-208.781	-133.569	19.461
1600	28.625	108.837	88.388	32.718	-208.457	-128.566	17.561
1700	28.900	110.581	89.643	35.594	-208.124	-123.580	15.887
1800	29.144	112.239	90.852	38.497	-207.784	-118.617	14.402
1900	29.361	113.821	92.020	41.422	-207.438	-113.672	13.075
2000	29.555	115.332	93.148	44.368	-207.090	-108.746	11.883

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 21.742 + 4.452\times10^{-3}T - 4.392\times10^{5}T^{-2}$

$H°- H°_{298} = 21.742\times10^{-3}T + 2.226\times10^{-6}T^{2} + 4.392\times10^{2}T^{-1} - 8.153$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -211.069 - 0.704\times10^{-3}T + 1.336\times10^{-6}T^{2} + 313.200T^{-1}$

$\Delta Gf° = -211.069 + 0.704\times10^{-3}T\ln T - 1.336\times10^{-6}T^{2} + 156.600T^{-1} + 48.401\times10^{-3}T$

Source: Data from Chase (24).

$(HF)_4(g)$

Tetrameric Hydrogen Fluoride (ideal gas)

[Formation: $2H_2(g) + 2F_2(g) = (HF)_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	25.474	83.437	83.437	0	-282.940	-260.321	190.818
300	25.540	83.595	83.438	.047	-282.947	-260.182	189.540
400	28.504	91.375	84.478	2.759	-283.161	-252.553	137.987
500	30.559	97.969	86.533	5.718	-283.208	-244.894	107.041
600	32.070	103.680	88.927	8.852	-283.134	-237.238	86.413
700	33.285	108.718	91.401	12.122	-282.964	-229.600	71.683
800	34.328	113.232	93.852	15.504	-282.718	-221.993	60.645
900	35.254	117.330	96.237	18.984	-282.402	-214.420	52.068
1000	36.084	121.088	98.537	22.551	-282.031	-206.889	45.215
1100	36.829	124.563	100.747	26.198	-281.608	-199.393	39.615
1200	37.493	127.796	102.868	29.914	-281.146	-191.938	34.956
1300	38.085	130.821	104.903	33.694	-280.648	-184.522	31.021
1400	38.611	133.663	106.857	37.529	-280.125	-177.151	27.654
1500	39.077	136.343	108.734	41.414	-279.580	-169.815	24.742
1600	39.491	138.879	110.540	45.343	-279.017	-162.516	22.198
1700	39.857	141.284	112.278	49.311	-278.439	-155.247	19.958
1800	40.183	143.572	113.954	53.313	-277.855	-148.021	17.972
1900	40.472	145.752	115.570	57.346	-277.260	-140.821	16.198
2000	40.731	147.835	117.132	61.407	-276.663	-133.657	14.605

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 30.316 + 5.934\times10^{-3}T - 5.877\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 30.316\times10^{-3}T + 2.967\times10^{-6}T^2 + 5.877\times10^{2}T^{-1} - 11.274$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -284.622 + 0.388\times10^{-3}T + 1.781\times10^{-6}T^2 + 419.700T^{-1}$

$\Delta Gf^\circ = -284.622 - 0.388\times10^{-3}T\ln T - 1.781\times10^{-6}T^2 + 209.850T^{-1} + 81.884\times10^{-3}T$

Source: Data from Chase (24).

$(HF)_5(g)$

Pentameric Hydrogen Fluoride (ideal gas)

[Formation: $2.5H_2(g) + 2.5F_2(g) = (HF)_5(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	32.820	97.594	97.594	0	-356.050	-325.779	238.799
300	32.903	97.797	97.594	.061	-356.056	-325.591	237.190
400	36.615	107.804	98.934	3.548	-356.227	-315.402	172.325
500	39.186	116.267	101.575	7.346	-356.186	-305.196	133.399
600	41.077	123.586	104.648	11.363	-355.994	-295.016	107.458
700	42.597	130.036	107.823	15.549	-355.683	-284.876	88.941
800	43.902	135.811	110.967	19.875	-355.277	-274.788	75.068
900	45.060	141.050	114.023	24.324	-354.783	-264.754	64.290
1000	46.098	145.852	116.969	28.883	-354.219	-254.784	55.682
1100	47.028	150.290	119.799	33.540	-353.592	-244.868	48.650
1200	47.859	154.419	122.514	38.286	-352.914	-235.013	42.801
1300	48.600	158.279	125.118	43.109	-352.193	-225.215	37.862
1400	49.257	161.905	127.617	48.003	-351.440	-215.479	33.637
1500	49.840	165.324	130.019	52.958	-350.659	-205.795	29.984
1600	50.356	168.558	132.328	57.968	-349.857	-196.166	26.795
1700	50.815	171.624	134.549	63.027	-349.035	-186.578	23.986
1800	51.222	174.541	136.691	68.130	-348.205	-177.049	21.496
1900	51.584	177.320	138.757	73.270	-347.362	-167.561	19.274
2000	51.906	179.974	140.751	78.445	-346.517	-158.120	17.278

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 38.884 + 7.420\times10^{-3}T - 7.358\times10^{-6}T^2$

$H°- H°_{298} = 38.884\times10^{-3}T + 3.710\times10^{-6}T^2 + 7.358\times10^{2}T^{-1} - 14.391$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -358.451 + 1.474\times10^{-3}T + 2.228\times10^{-6}T^2 + 525.800T^{-1}$

$\Delta Gf° = -358.451 - 1.474\times10^{-3}T\ln T - 2.228\times10^{-6}T^2 + 262.900T^{-1} + 115.689\times10^{-3}T$

Source: Data from Chase (24).

$(HF)_6(g)$

Hexameric Hydrogen Fluoride (ideal gas)

[Formation: $3H_2(g) + 3F_2(g) = (HF)_6(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	40.166	111.451	111.451	0	-432.040	-394.026	288.825
300	40.265	111.700	111.453	.074	-432.047	-393.792	286.874
400	44.726	123.934	113.089	4.338	-432.172	-381.009	208.171
500	47.813	134.266	116.318	8.974	-432.045	-368.230	160.951
600	50.084	143.193	120.070	13.874	-431.735	-355.494	129.487
700	51.909	151.055	123.946	18.976	-431.283	-342.822	107.032
800	53.475	158.091	127.782	24.247	-430.716	-330.223	90.212
900	54.865	164.471	131.510	29.665	-430.044	-317.699	77.147
1000	56.111	170.317	135.102	35.215	-429.288	-305.260	66.714
1100	57.228	175.719	138.553	40.883	-428.456	-292.895	58.192
1200	58.225	180.742	141.861	46.657	-427.563	-280.609	51.105
1300	59.114	185.438	145.035	52.524	-426.619	-268.399	45.121
1400	59.903	189.848	148.079	58.476	-425.635	-256.269	40.005
1500	60.602	194.005	151.004	64.502	-424.619	-244.206	35.580
1600	61.222	197.937	153.816	70.594	-423.576	-232.214	31.719
1700	61.772	201.665	156.521	76.744	-422.511	-220.279	28.318
1800	62.260	205.210	159.129	82.946	-421.436	-208.419	25.305
1900	62.695	208.588	161.644	89.194	-420.345	-196.610	22.615
2000	63.082	211.814	164.072	95.483	-419.252	-184.866	20.201

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 47.077 + 9.208\times10^{-3}T - 8.584\times10^{5}T^{-2}$

$H°- H°_{298} = 47.077\times10^{-3}T + 4.604\times10^{-6}T^2 + 8.584\times10^{2}T^{-1} - 17.324$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -434.976 + 2.185\times10^{-3}T + 2.825\times10^{-6}T^2 + 606.400T^{-1}$

$\Delta Gf° = -434.976 - 2.185\times10^{-3}T\ln T - 2.825\times10^{-6}T^2 + 303.200T^{-1} + 147.229\times10^{-3}T$

Source: Data from Chase (24).

$(HF)_7(g)$

Heptameric Hydrogen Fluoride (ideal gas)

[Formation: $3.5H_2(g) + 3.5F_2(g) = (HF)_7(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	47.512	125.077	125.077	0	-502.520	-456.695	334.762
300	47.628	125.371	125.078	.088	-502.526	-456.412	332.492
400	52.836	139.833	127.015	5.127	-502.608	-441.015	240.956
500	56.441	152.034	130.830	10.602	-502.393	-425.637	186.044
600	59.091	162.569	135.262	16.384	-501.966	-410.325	149.459
700	61.221	171.843	139.839	22.403	-501.372	-395.096	123.353
800	63.049	180.139	144.367	28.618	-500.645	-379.963	103.800
900	64.670	187.661	148.765	35.006	-499.794	-364.925	88.615
1000	66.124	194.551	153.004	41.547	-498.846	-349.995	76.490
1100	67.427	200.916	157.074	48.226	-497.809	-335.157	66.589
1200	68.591	206.834	160.977	55.028	-496.702	-320.417	58.355
1300	69.628	212.366	164.720	61.940	-495.533	-305.771	51.404
1400	70.548	217.560	168.311	68.949	-494.320	-291.225	45.462
1500	71.364	222.456	171.759	76.046	-493.069	-276.762	40.324
1600	72.088	227.085	175.073	83.219	-491.786	-262.384	35.840
1700	72.729	231.475	178.263	90.461	-490.477	-248.078	31.892
1800	73.299	235.648	181.335	97.763	-489.156	-233.861	28.394
1900	73.806	239.625	184.300	105.118	-487.818	-219.711	25.272
2000	74.258	243.423	187.162	112.522	-486.475	-205.638	22.471

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 55.586 + 10.742\times10^{-3}T - 10.025\times10^{5}T^{-2}$

$H°- H°_{298} = 55.586\times10^{-3}T + 5.371\times10^{-6}T^{2} + 10.025\times10^{2}T^{-1} - 20.413$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -506.147 + 3.212\times10^{-3}T + 3.296\times10^{-6}T^{2} + 708.500T^{-1}$

$\Delta Gf° = -506.147 - 3.212\times10^{-3}T\ln T - 3.296\times10^{-6}T^{2} + 354.250T^{-1} + 181.161\times10^{-3}T$

Source: Data from Chase (24).

HI(g)

Hydrogen Iodide (ideal gas)

[Formation: $0.5H_2(g) + 0.5I_2(c,l,g) = HI(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	6.969	49.350	49.350	0	6.300	.377	-.276
300	6.969	49.393	49.350	.013	6.295	.340	-.248
386.8	7.005	51.167	49.568	.619	5.995	-1.346	.760
386.8	7.005	51.167	49.568	.619	4.140	-1.346	.760
400	7.010	51.402	49.625	.711	4.060	-1.531	.837
458.4	7.067	52.360	49.912	1.122	3.704	-2.322	1.107
458.4	7.067	52.360	49.912	1.122	-1.306	-2.322	1.107
500	7.107	52.976	50.142	1.417	-1.343	-2.411	1.054
600	7.253	54.284	50.727	2.134	-1.425	-2.618	.954
700	7.424	55.415	51.318	2.868	-1.491	-2.812	.878
800	7.600	56.418	51.893	3.620	-1.542	-2.995	.818
900	7.767	57.323	52.447	4.388	-1.582	-3.175	.771
1000	7.920	58.149	52.977	5.172	-1.609	-3.351	.732
1100	8.056	58.910	53.482	5.971	-1.627	-3.524	.700
1200	8.177	59.616	53.964	6.783	-1.637	-3.695	.673
1300	8.283	60.275	54.424	7.606	-1.642	-3.866	.650
1400	8.376	60.893	54.865	8.439	-1.643	-4.038	.630
1500	8.459	61.473	55.286	9.281	-1.641	-4.209	.613
1600	8.531	62.022	55.690	10.131	-1.637	-4.381	.598
1700	8.596	62.541	56.078	10.987	-1.632	-4.552	.585
1800	8.654	63.034	56.451	11.850	-1.626	-4.724	.574
1900	8.706	63.503	56.809	12.718	-1.620	-4.895	.563
2000	8.753	63.951	57.156	13.591	-1.615	-5.068	.554
2100	8.796	64.379	57.489	14.468	-1.610	-5.241	.545
2200	8.835	64.789	57.812	15.350	-1.605	-5.415	.538
2300	8.871	65.183	58.124	16.235	-1.602	-5.589	.531
2400	8.904	65.561	58.426	17.124	-1.599	-5.761	.525
2500	8.935	65.925	58.719	18.016	-1.597	-5.934	.519
2600	8.963	66.276	59.003	18.911	-1.596	-6.108	.513
2700	8.990	66.615	59.279	19.808	-1.596	-6.282	.509
2800	9.016	66.942	59.546	20.709	-1.597	-6.454	.504
2900	9.040	67.259	59.807	21.611	-1.600	-6.629	.500
3000	9.062	67.566	60.060	22.517	-1.603	-6.802	.496

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 6.607 + 1.200\times10^{-3}T$

$H°- H°_{298} = 6.607\times10^{-3}T + 0.600\times10^{-6}T^2 - 2.023$

2000-3000 K: $Cp° = 8.672 + 0.172\times10^{-3}T - 10.560\times10^{5}T^{-2}$

$H°- H°_{298} = 8.672\times10^{-3}T + 0.086\times10^{-6}T^2 + 10.560\times10^{2}T^{-1} - 4.625$

HI(g) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = 7.216 - 3.059\times10^{-3}T - 0.355\times10^{-6}T^2 + 8.250T^{-1}$

$\Delta Gf^\circ = 7.216 + 3.059\times10^{-3}T\ln T + 0.355\times10^{-6}T^2 + 4.125T^{-1} - 40.524\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = 6.489 - 6.262\times10^{-3}T + 0.391\times10^{-6}T^2 + 8.250T^{-1}$

$\Delta Gf^\circ = 6.489 + 6.262\times10^{-3}T\ln T - 0.391\times10^{-6}T^2 + 4.125T^{-1} - 57.432\times10^{-3}T$

458.4-2000 K: $\Delta Hf^\circ = -0.868 - 1.092\times10^{-3}T + 0.356\times10^{-6}T^2 + 0.600T^{-1}$

$\Delta Gf^\circ = -0.868 + 1.092\times10^{-3}T\ln T - 0.356\times10^{-6}T^2 + 0.300T^{-1} - 9.701\times10^{-3}T$

2000-3000 K: $\Delta Hf^\circ = -3.470 + 0.973\times10^{-3}T - 0.158\times10^{-6}T^2 + 1056.600T^{-1}$

$\Delta Gf^\circ = -3.470 - 0.973\times10^{-3}T\ln T + 0.158\times10^{-6}T^2 + 528.300T^{-1} + 6.136\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 from CODATA (34). Other data from JANAF (60).

$HfBr_4(c)$

Hafnium Tetrabromide

[Formation: $Hf(c) + 2Br_2(1,g) = HfBr_4(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	30.500	57.000	57.000	0	-183.140	-175.338	128.525
300	30.530	57.190	57.007	.055	-183.162	-175.289	127.697
332.6	31.022	60.365	57.183	1.058	-183.536	-174.415	114.606
332.6	31.022	60.365	57.183	1.058	-197.666	-174.415	114.606
400	32.040	66.180	58.217	3.185	-197.141	-169.759	92.751
500	33.560	73.490	60.560	6.465	-196.267	-163.008	71.250
600	35.080	79.740	63.248	9.895	-195.274	-156.449	56.986
700	36.590	85.270	66.013	13.480	-194.154	-150.068	46.853

*Data except enthalpy of formation at 298 K estimated.

Phase change: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp^\circ = 25.980 + 15.160\times10^{-3}T$

$H^\circ - H^\circ_{298} = 25.980\times10^{-3}T + 7.580\times10^{-6}T^2 - 8.420$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -179.037 - 15.811\times10^{-3}T + 6.870\times10^{-6}T^2$

$\Delta Gf^\circ = -179.037 + 15.811\times10^{-3}T\ln T - 6.870\times10^{-6}T^2 - 75.631\times10^{-3}T$

332.6-700 K: $\Delta Hf^\circ = -199.037 + 2.511\times10^{-3}T + 6.560\times10^{-6}T^2 - 62.800T^{-1}$

$\Delta Gf^\circ = -199.037 - 2.511\times10^{-3}T\ln T - 6.560\times10^{-6}T^2 - 31.400T^{-1} + 91.079\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Vasil'ev (248). Entropy at 298 K estimated by Kelley (118). High-temperature data are those estimated by Kelley (117).

$HfBr_4(g)$

Hafnium Tetrabromide (ideal gas)

[Formation: $Hf(c) + 2Br_2(l,g) = HfBr_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	24.750	100.100	100.100	0	-157.000	-162.048	118.783
300	24.760	100.260	100.107	.046	-157.031	-162.079	118.073
332.6	24.907	102.822	100.249	.856	-157.599	-162.599	106.842
332.6	24.907	102.822	100.249	.856	-171.729	-162.599	106.842
400	25.210	107.450	101.080	2.548	-171.638	-160.764	87.836
500	25.430	113.100	102.938	5.081	-171.511	-158.057	69.086
600	25.550	117.750	105.033	7.630	-171.399	-155.380	56.596
700	25.620	121.690	107.133	10.190	-171.304	-152.712	47.678
800	25.670	125.120	109.176	12.755	-171.227	-150.065	40.995
900	25.710	128.150	111.123	15.324	-171.171	-147.431	35.801
1000	25.730	130.860	112.964	17.896	-171.133	-144.799	31.645

*Enthalpy of formation at 298 K estimated.

Phase change: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 25.776 + 0.050\times10^{-3}T - 0.925\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.776\times10^{-3}T + 0.025\times10^{-6}T^2 + 0.925\times10^{2}T^{-1} - 7.998$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -152.474 - 16.015\times10^{-3}T - 0.685\times10^{-6}T^2 + 92.500T^{-1}$

$\Delta Gf^\circ = -152.474 + 16.015\times10^{-3}T\ln T + 0.685\times10^{-6}T^2 + 46.250T^{-1} - 124.082\times10^{-3}T$

332.6-1000 K: $\Delta Hf^\circ = -172.475 + 2.307\times10^{-3}T - 0.995\times10^{-6}T^2 + 29.700T^{-1}$

$\Delta Gf^\circ = -172.475 - 2.307\times10^{-3}T\ln T + 0.995\times10^{-6}T^2 + 14.850T^{-1} + 42.628\times10^{-3}T$

Sources: Enthalpy of formation at 298 K estimated. Other data from Clark (31).

$HfCl_4(c,g)$

Hafnium Tetrachloride

[Formation: $Hf(c) + 2Cl_2(g) = HfCl_4(c,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	28.800	45.570	45.570	0	-236.700	-215.406	157.895
300	28.829	45.748	45.571	.053	-236.688	-215.273	156.825
400	29.935	54.216	46.718	2.999	-236.027	-208.237	113.774
500	30.505	60.962	48.914	6.024	-235.350	-201.362	88.014
589	30.835	65.987	51.126	8.753	-234.754	-195.367	72.490
589	25.200	105.763	51.126	32.181	-211.326	-195.367	72.490
600	25.230	106.230	52.133	32.458	-211.315	-195.069	71.053
700	25.380	110.130	60.144	34.990	-211.218	-192.366	60.058
800	25.490	113.530	66.613	37.534	-211.144	-189.683	51.818
900	25.560	116.530	71.990	40.086	-211.087	-186.999	45.409
1000	25.610	119.230	76.585	42.645	-211.050	-184.334	40.286

Phase change: 589 K, sublimation point of $HfCl_4$; ΔH° = 23.428 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-589 K: $Cp^\circ = 30.873 + 0.926\times10^{-3}T - 2.086\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 30.873\times10^{-3}T + 0.463\times10^{-6}T^2 + 2.086\times10^{2}T^{-1} - 9.946$

589-1000 K: $Cp^\circ = 25.953 - 0.110\times10^{-3}T - 2.385\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.953\times10^{-3}T - 0.055\times10^{-6}T^2 + 2.385\times10^{2}T^{-1} + 16.509$

Formation equations (kcal/mol):

298.15-589 K: $\Delta Hf^\circ = -239.155 + 7.610\times10^{-3}T - 0.623\times10^{-6}T^2 + 72.000T^{-1}$

$\Delta Gf^\circ = -239.155 - 7.610\times10^{-3}T\ln T + 0.623\times10^{-6}T^2 + 36.000T^{-1} + 122.422\times10^{-3}T$

589-1000 K: $\Delta Hf^\circ = -212.700 + 2.690\times10^{-3}T - 1.141\times10^{-6}T^2 + 101.900T^{-1}$

$\Delta Gf^\circ = -212.700 - 2.690\times10^{-3}T\ln T + 1.141\times10^{-6}T^2 + 50.950T^{-1} + 45.777\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (254). Low-temperature heat capacities and entropy at 298 K from Todd (240). High-temperature data of crystal based on Orr (176). See $HfCl_4(g)$ for sources of gas data.

$HfCl_4(g)$

Hafnium Tetrachloride (ideal gas)

[Formation: $Hf(c) + 2Cl_2(g) = HfCl_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	23.650	89.030	89.030	0	-211.690	-203.354	149.060
300	23.670	89.180	89.033	.044	-211.687	-203.302	148.104
400	24.540	96.120	89.973	2.459	-211.557	-200.529	109.563
500	24.980	101.650	91.776	4.937	-211.427	-197.783	86.450
600	25.230	106.230	93.817	7.448	-211.315	-195.069	71.053
700	25.380	110.130	95.873	9.980	-211.218	-192.366	60.058
800	25.490	113.530	97.875	12.524	-211.144	-189.683	51.818
900	25.560	116.530	99.779	15.076	-211.087	-186.999	45.409
1000	25.610	119.230	101.595	17.635	-211.050	-184.334	40.286

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 25.531 + 0.282\times10^{-3}T - 1.747\times10^{5}T^{-2}$

$H°- H°_{298} = 25.531\times10^{-3}T + 0.141\times10^{-6}T^{2} + 1.747\times10^{2}T^{-1} - 8.211$

Formation equations (kcal/mol):

298.15-1000 K: $\Delta Hf° = -212.410 + 2.268\times10^{-3}T - 0.945\times10^{-6}T^{2} + 38.100T^{-1}$

$\Delta Gf° = -212.410 - 2.268\times10^{-3}T\ln T + 0.945\times10^{-6}T^{2} + 19.050T^{-1} + 42.801\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Palko (182) and Izmailovich (107). Other data from Clark (31).

HfF_4(c,g)

Hafnium Tetrafluoride

[Formation: $Hf(c) + 2F_2(g) = HfF_4(c,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	24.000	27.000	27.000	0	-461.400	-437.460	320.663
300	24.080	27.149	27.002	.044	-461.395	-437.311	318.577
400	27.042	34.537	27.987	2.620	-460.982	-429.341	234.578
500	28.610	40.755	29.937	5.409	-460.443	-421.487	184.230
600	29.635	46.067	32.194	8.324	-459.849	-413.755	150.708
700	30.405	50.695	34.512	11.328	-459.220	-406.119	126.794
800	31.038	54.798	36.797	14.401	-458.569	-398.580	108.886
900	31.592	58.486	39.005	17.533	-457.894	-391.121	94.976
1000	32.096	61.841	41.124	20.717	-457.204	-383.745	83.866
1100	32.569	64.923	43.149	23.951	-456.494	-376.428	74.788
1200	33.019	67.776	45.084	27.230	-455.767	-369.182	67.236
1235.5	33.175	68.741	45.752	28.403	-455.507	-366.627	64.852
1235.5	25.527	114.883	45.752	85.411	-398.499	-366.627	64.852
1300	25.570	116.183	49.215	87.059	-398.517	-364.963	61.355
1400	25.641	118.081	54.067	89.619	-398.563	-362.380	56.569
1500	25.720	119.852	58.394	92.187	-398.626	-359.791	52.421

*Heat capacity at 298 K and gas data estimated.

Phase change: 1235.5 K, calculated sublimation point of HfF_4; ΔH° = 57.008 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1235.5 K: $Cp^\circ = 28.852 + 3.774\times10^{-3}T - 5.313\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 28.852\times10^{-3}T + 1.887\times10^{-6}T^2 + 5.313\times10^{2}T^{-1} - 10.552$

1235.5-1500 K: $Cp^\circ = 25.140 + 0.456\times10^{-3}T - 2.676\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.140\times10^{-3}T + 0.228\times10^{-6}T^2 + 2.676\times10^{2}T^{-1} + 53.786$

Formation equations (kcal/mol):

298.15-1235.5 K: $\Delta Hf^\circ = -464.420 + 6.227\times10^{-3}T + 0.629\times10^{-6}T^2 + 330.300T^{-1}$

$\Delta Gf^\circ = -464.420 - 6.227\times10^{-3}T\ln T - 0.629\times10^{-6}T^2 + 165.150T^{-1} + 124.235\times10^{-3}T$

1235.5-1500 K: $\Delta Hf^\circ = -400.080 + 2.515\times10^{-3}T - 1.030\times10^{-6}T^2 + 66.600T^{-1}$

$\Delta Gf^\circ = -400.080 - 2.515\times10^{-3}T\ln T + 1.030\times10^{-6}T^2 + 33.300T^{-1} + 43.769\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (254). Heat capacity at 298 K estimated. High-temperature data based on Kaylor (114) and Smith (217). Enthalpy of formation at 298 K for gas from Wagman (254). Other gas data estimated.

$HfF_4(g)$

Hafnium Tetrafluoride (ideal gas)

[Formation: $Hf(c) + 2F_2(g) = HfF_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	21.760	80.385	80.385	0	-399.100	-391.076	286.663
300	21.797	80.520	80.387	.040	-399.099	-391.027	284.859
400	23.244	87.010	81.260	2.300	-399.002	-388.350	212.182
500	24.057	92.292	82.954	4.669	-398.883	-385.696	168.585
600	24.555	96.726	84.891	7.101	-398.772	-383.074	139.533
700	24.876	100.537	86.860	9.574	-398.674	-380.462	118.784
800	25.091	103.874	88.783	12.073	-398.597	-377.869	103.228
900	25.240	106.838	90.627	14.590	-398.537	-375.281	91.130
1000	25.348	109.503	92.384	17.119	-398.502	-372.705	81.454
1100	25.432	111.923	94.052	19.658	-398.487	-370.121	73.535
1200	25.503	114.139	95.635	22.205	-398.492	-367.543	66.938
1300	25.570	116.183	97.138	24.759	-398.517	-364.963	61.355
1400	25.641	118.081	98.567	27.319	-398.563	-362.380	56.569
1500	25.720	119.852	99.927	29.887	-398.626	-359.791	52.421

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp^\circ = 25.055 + 0.556\times10^{-3}T - 3.077\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.055\times10^{-3}T + 0.278\times10^{-6}T^2 + 3.077\times10^{2}T^{-1} - 8.527$

Formation equations (kcal/mol):

298.15-1500 K: $\Delta Hf^\circ = -400.095 + 2.430\times10^{-3}T - 0.980\times10^{-6}T^2 + 106.700T^{-1}$

$\Delta Gf^\circ = -400.095 - 2.430\times10^{-3}T\ln T + 0.980\times10^{-6}T^2 + 53.350T^{-1} + 43.202\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (254). Other data estimated.

HfI_4(c)

Hafnium Tetraiodide

[Formation: $Hf(c) + 2I_2(c,l,g) = HfI_4(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	34.500	64.500	64.500	0	-118.000	-117.575	86.184
300	34.510	64.710	64.500	.065	-117.994	-117.569	85.648
386.8	35.152	73.559	65.582	3.085	-117.931	-117.467	66.371
386.8	35.152	73.559	65.582	3.085	-125.349	-117.467	66.371
400	35.250	74.740	65.865	3.550	-125.478	-117.196	64.032
458.4	35.688	79.576	67.308	5.624	-126.026	-115.940	55.275
458.4	35.688	79.576	67.308	5.624	-146.068	-115.940	55.275
500	36.000	82.690	68.460	7.115	-145.591	-113.223	49.489
600	36.750	89.320	71.403	10.750	-144.411	-106.867	38.926
700	37.500	95.040	74.376	14.465	-143.173	-100.700	31.439
800	38.240	100.100	77.287	18.250	-141.888	-94.725	25.877

*Data estimated.

Phase changes: 386.4 K, melting point of I_2: $\Delta H° = 3.709$ kcal/mol.
458.4 K, boiling point of I_2; $\Delta H° = 10.021$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp° = 32.270 + 7.460\times10^{-3}T$

$H°- H°_{298} = 32.270\times10^{-3}T + 3.730\times10^{-6}T^2 - 9.953$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -118.256 + 0.907\times10^{-3}T - 0.164\times10^{-6}T^2$

$\Delta Gf° = -118.256 - 0.907\times10^{-3}T\ln T + 0.164\times10^{-6}T^2 + 7.403\times10^{-3}T$

386.8-458.4 K: $\Delta Hf° = -121.166 - 11.901\times10^{-3}T + 2.820\times10^{-6}T^2$

$\Delta Gf° = -121.166 + 11.901\times10^{-3}T\ln T - 2.820\times10^{-6}T^2 - 60.228\times10^{-3}T$

458.4-800 K: $\Delta Hf° = -150.593 + 8.779\times10^{-3}T + 2.684\times10^{-6}T^2 - 30.600T^{-1}$

$\Delta Gf° = -150.593 - 8.779\times10^{-3}T\ln T - 2.684\times10^{-6}T^2 - 15.300T^{-1} + 130.698\times10^{-3}T$

Sources: Enthalpy of formation at 298 K estimated by Spencer (224). Entropy at 298 K estimated by Kelley (118). High-temperature data are those estimated by Kelley (117).

$HfI_4(g)$

Hafnium Tetraiodide (ideal gas)

[Formation: $Hf(c) + 2I_2(c,l,g) = HfI_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	25.120	105.940	105.940	0	-87.000	-98.930	72.517
300	25.130	106.090	105.940	.046	-87.013	-99.002	72.122
386.8	25.390	112.517	106.722	2.242	-87.775	-102.380	57.846
386.8	25.390	112.517	106.722	2.242	-95.193	-102.380	57.846
400	25.430	113.370	106.928	2.577	-95.451	-102.621	56.069
458.4	25.512	116.841	107.975	4.064	-96.586	-103.581	49.383
458.4	25.512	116.841	107.975	4.064	-116.628	-103.581	49.383
500	25.570	119.060	108.806	5.127	-116.579	-102.396	44.757
600	25.650	123.730	110.915	7.689	-116.472	-99.574	36.269
700	25.700	127.690	113.037	10.257	-116.381	-96.763	30.210
800	25.730	131.120	115.085	12.828	-116.310	-93.963	25.669
900	25.750	134.150	117.037	15.402	-116.259	-91.174	22.140
1000	25.770	136.870	118.892	17.978	-116.227	-88.397	19.319

*Enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 25.820 + 0.006\times10^{-3}T - 0.624\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.820\times10^{-3}T + 0.003\times10^{-6}T^2 + 0.624\times10^{2}T^{-1} - 7.908$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -85.211 - 5.543\times10^{-3}T - 3.891\times10^{-6}T^2 + 62.400T^{-1}$

$\Delta Gf^\circ = -85.211 + 5.543\times10^{-3}T\ln T + 3.891\times10^{-6}T^2 + 31.200T^{-1} - 79.108\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -88.121 - 18.351\times10^{-3}T - 0.907\times10^{-6}T^2 + 62.400T^{-1}$

$\Delta Gf^\circ = -88.121 + 18.351\times10^{-3}T\ln T + 0.907\times10^{-6}T^2 + 31.200T^{-1} - 146.739\times10^{-3}T$

458.4-1000 K: $\Delta Hf^\circ = -117.547 + 2.329\times10^{-3}T - 1.043\times10^{-6}T^2 + 31.800T^{-1}$

$\Delta Gf^\circ = -117.547 - 2.329\times10^{-3}T\ln T + 1.043\times10^{-6}T^2 + 15.900T^{-1} + 44.187\times10^{-3}T$

Sources: Enthalpy of formation at 298 K estimated. Other data from Clark (31).

HgBr(g)

Mercury Monobromide (ideal gas)

[Formation: $Hg(l,g) + 0.5Br_2(l,g) = HgBr(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.894	64.875	64.875	0	24.900	16.389	-12.013
300	8.896	64.930	64.877	.016	24.888	16.336	-11.901
332.6	8.923	65.849	64.928	.306	24.667	15.419	-10.131
332.6	8.923	65.849	64.928	.306	21.134	15.419	-10.131
400	8.978	67.502	65.227	.910	21.000	14.272	-7.798
500	9.031	69.511	65.889	1.811	20.808	12.613	-5.513
600	9.072	71.161	66.634	2.716	20.619	10.991	-4.003
629.81	9.083	71.601	66.859	2.987	20.564	10.516	-3.649
629.81	9.083	71.601	66.859	2.987	6.413	10.516	-3.649
700	9.108	72.562	67.383	3.625	6.390	10.975	-3.427
800	9.140	73.781	68.108	4.538	6.358	11.632	-3.178
900	9.171	74.859	68.800	5.453	6.327	12.293	-2.985
1000	9.201	75.827	69.455	6.372	6.299	12.957	-2.832
1100	9.230	76.705	70.074	7.294	6.273	13.624	-2.707
1200	9.259	77.510	70.662	8.218	6.249	14.293	-2.603
1300	9.287	78.252	71.217	9.145	6.227	14.964	-2.516
1400	9.315	78.941	71.745	10.075	6.207	15.639	-2.441
1500	9.343	79.585	72.246	11.008	6.189	16.311	-2.376
1600	9.371	80.189	72.724	11.944	6.174	16.987	-2.320
1700	9.398	80.758	73.180	12.883	6.160	17.663	-2.271
1800	9.426	81.296	73.616	13.824	6.150	18.341	-2.227
1900	9.453	81.806	74.033	14.768	6.141	19.020	-2.188
2000	9.481	82.291	74.434	15.714	6.133	19.698	-2.152

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
629.81 K, boiling point of Hg; ΔH° = 14.151 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.938 + 0.274\times10^{-3}T - 0.111\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.938\times10^{-3}T + 0.137\times10^{-6}T^2 + 0.111\times10^{2}T^{-1} - 2.714$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = 26.652 - 6.380\times10^{-3}T + 0.086\times10^{-6}T^2 + 42.500T^{-1}$

$\Delta Gf^\circ = 26.652 + 6.380\times10^{-3}T\ln T - 0.086\times10^{-6}T^2 + 21.250T^{-1} - 70.989\times10^{-3}T$

332.6-629.81 K: $\Delta Hf^\circ = 21.652 - 1.800\times10^{-3}T + 0.008\times10^{-6}T^2 + 26.800T^{-1}$

$\Delta Gf^\circ = 21.652 + 1.800\times10^{-3}T\ln T - 0.008\times10^{-6}T^2 + 13.400T^{-1} - 29.312\times10^{-3}T$

629.81-2000 K: $\Delta Hf^\circ = 6.689 - 0.495\times10^{-3}T + 0.109\times10^{-6}T^2 - 4.600T^{-1}$

$\Delta Gf^\circ = 6.689 + 0.495\times10^{-3}T\ln T - 0.109\times10^{-6}T^2 - 2.300T^{-1} + 2.961\times10^{-3}T$

Source: Data from JANAF (60) who estimated some molecular constants.

$Hg_2Br_2(c)$

Dimeric Mercury Monobromide

[Formation: $2Hg(l) + Br_2(l,g) = Hg_2Br_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	25.000	52.283	52.283	0	-49.450	-43.375	31.794
300	25.025	52.438	52.285	.046	-49.461	-43.336	31.570
332.6	25.408	55.039	52.429	.868	-49.661	-42.661	28.032
332.6	25.408	55.039	52.429	.868	-56.726	-42.661	28.032
400	26.200	59.805	53.280	2.610	-56.461	-39.837	21.766
500	27.020	65.744	55.198	5.273	-55.984	-35.735	15.620
600	27.630	70.726	57.381	8.007	-55.436	-31.736	11.560

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.

666 K, vapor pressure of decomposition products, Hg(g) and $HgBr_2(g)$ = 1 atm.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp^\circ = 25.026 + 5.030\times10^{-3}T - 1.356\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.026\times10^{-3}T + 2.515\times10^{-6}T^2 + 1.356\times10^{2}T^{-1} - 8.140$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -48.657 - 5.611\times10^{-3}T + 2.413\times10^{-6}T^2 + 198.400T^{-1}$

$\Delta Gf^\circ = -48.657 + 5.611\times10^{-3}T\ln T - 2.413\times10^{-6}T^2 + 99.200T^{-1} - 14.649\times10^{-3}T$

332.6-600 K: $\Delta Hf^\circ = -58.657 + 3.550\times10^{-3}T + 2.258\times10^{-6}T^2 + 167.000T^{-1}$

$\Delta Gf^\circ = -58.657 - 3.550\times10^{-3}T\ln T - 2.258\times10^{-6}T^2 + 83.500T^{-1} + 68.706\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (253). Other data are those estimated by JANAF (60).

$HgBr_2$(c,l,g)
Mercury Dibromide
[Formation: $Hg(l,g) + Br_2(l,g) = HgBr_2(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	18.000	40.706	40.706	0	-41.900	-37.782	27.694
300	18.013	40.817	40.707	.033	-41.912	-37.755	27.505
332.6	18.242	42.687	40.811	.624	-42.126	-37.293	24.505
332.6	18.242	42.687	40.811	.624	-49.191	-37.293	24.505
400	18.714	46.095	41.420	1.870	-48.978	-34.904	19.070
500	19.414	50.347	42.795	3.776	-48.606	-31.428	13.737
514	19.512	50.883	43.004	4.050	-48.547	-30.946	13.158
514	24.400	59.210	43.004	8.330	-44.267	-30.946	13.158
592	24.400	62.655	45.369	10.233	-43.563	-28.974	10.696
592	14.770	86.545	45.369	24.376	-29.420	-28.974	10.696
600	14.774	86.741	45.911	24.498	-29.421	-28.963	10.549
629.81	14.784	87.458	47.861	24.939	-29.439	-28.937	10.041
629.81	14.784	87.458	47.861	24.939	-43.590	-28.937	10.041
700	14.808	89.021	51.911	25.977	-43.527	-27.307	8.526
800	14.830	91.000	56.676	27.459	-43.437	-24.996	6.829
900	14.846	92.748	60.589	28.943	-43.349	-22.697	5.511
1000	14.857	94.313	63.885	30.428	-43.261	-20.408	4.460
1100	14.865	95.729	66.716	31.914	-43.174	-18.127	3.601
1200	14.871	97.023	69.189	33.401	-43.087	-15.853	2.887
1300	14.876	98.213	71.376	34.888	-43.001	-13.587	2.284
1400	14.880	99.316	73.333	36.376	-42.916	-11.326	1.768
1500	14.883	100.343	75.100	37.864	-42.833	-9.076	1.322
1600	14.886	101.303	76.707	39.353	-42.750	-6.825	.932
1700	14.888	102.206	78.182	40.841	-42.669	-4.586	.590
1800	14.890	103.057	79.540	42.330	-42.587	-2.346	.285
1900	14.891	103.862	80.799	43.819	-42.507	-.110	.013
2000	14.893	104.626	81.972	45.309	-42.428	2.118	-.231

*Entropy at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
514 K, melting point of $HgBr_2$; ΔH° = 4.280 kcal/mol.
592 K, boiling point of $HgBr_2$; ΔH° = 14.143 kcal/mol.
629.81 K, boiling point of Hg; ΔH° = 14.151 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-514 K: $Cp^\circ = 15.904 + 7.050\times10^{-3}T - 0.005\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 15.904\times10^{-3}T + 3.525\times10^{-6}T^2 + 0.005\times10^{2}T^{-1} - 5.057$

514-592 K: $Cp^\circ = 24.400$

$H^\circ - H^\circ_{298} = 24.400\times10^{-3}T - 4.212$

592-2000 K: $Cp^\circ = 15.012 - 0.070\times10^{-3}T - 0.703\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 15.012\times10^{-3}T - 0.035\times10^{-6}T^2 + 0.703\times10^{2}T^{-1} + 15.382$

$HgBr_2$(c,l,g) - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -39.798 - 8.460\times10^{-3}T + 3.524\times10^{-6}T^2 + 31.900T^{-1}$

$\Delta Gf^\circ = -39.798 + 8.460\times10^{-3}T\ln T - 3.524\times10^{-6}T^2 + 15.950T^{-1} - 40.568\times10^{-3}T$

332.6-514 K: $\Delta Hf^\circ = -49.798 + 0.701\times10^{-3}T + 3.369\times10^{-6}T^2 + 0.500T^{-1}$

$\Delta Gf^\circ = -49.798 - 0.701\times10^{-3}T\ln T - 3.369\times10^{-6}T^2 + 0.250T^{-1} + 42.787\times10^{-3}T$

514-592 K: $\Delta Hf^\circ = -48.953 + 9.197\times10^{-3}T - 0.156\times10^{-6}T^2$

$\Delta Gf^\circ = -48.953 - 9.197\times10^{-3}T\ln T + 0.156\times10^{-6}T^2 + 92.366\times10^{-3}T$

592-629.81 K: $\Delta Hf^\circ = -29.359 - 0.191\times10^{-3}T - 0.191\times10^{-6}T^2 + 70.300T^{-1}$

$\Delta Gf^\circ = -29.359 + 0.191\times10^{-3}T\ln T + 0.191\times10^{-6}T^2 + 35.150T^{-1} - 0.782\times10^{-3}T$

629.81-2000 K: $\Delta Hf^\circ = -44.322 + 1.114\times10^{-3}T - 0.090\times10^{-6}T^2 + 38.900T^{-1}$

$\Delta Gf^\circ = -44.322 - 1.114\times10^{-3}T\ln T + 0.090\times10^{-6}T^2 + 19.450T^{-1} + 31.491\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Vasil´ev (247). Other data from JANAF (60) who estimated entropy at 298 K.

$HgBr_2(g)$

Mercury Dibromide (ideal gas)

[Formation: $Hg(l,g) + Br_2(l,g) = HgBr_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	14.407	76.511	76.511	0	-21.824	-28.381	20.804
300	14.412	76.600	76.511	.027	-21.842	-28.420	20.704
332.6	14.479	78.090	76.593	.498	-22.176	-29.118	19.133
332.6	14.479	78.090	76.593	.498	-29.241	-29.118	19.133
400	14.618	80.779	77.079	1.480	-29.292	-29.091	15.894
500	14.718	84.052	78.158	2.947	-29.359	-29.033	12.690
600	14.774	86.741	79.371	4.422	-29.421	-28.963	10.549
629.81	14.784	87.458	79.737	4.863	-29.439	-28.937	10.041
629.81	14.784	87.458	79.737	4.863	-43.590	-28.937	10.041
700	14.808	89.021	80.591	5.901	-43.527	-27.307	8.526
800	14.830	91.000	81.771	7.383	-43.437	-24.996	6.829
900	14.846	92.748	82.896	8.867	-43.349	-22.697	5.511
1000	14.857	94.313	83.961	10.352	-43.261	-20.408	4.460
1100	14.865	95.729	84.967	11.838	-43.174	-18.127	3.601
1200	14.871	97.023	85.919	13.325	-43.087	-15.853	2.887
1300	14.876	98.213	86.819	14.812	-43.001	-13.587	2.284
1400	14.880	99.316	87.673	16.300	-42.916	-11.326	1.768
1500	14.883	100.343	88.484	17.788	-42.833	-9.076	1.322
1600	14.886	101.303	89.255	19.277	-42.750	-6.825	.932
1700	14.888	102.206	89.991	20.765	-42.669	-4.586	.590
1800	14.890	103.057	90.694	22.254	-42.587	-2.346	.285
1900	14.891	103.862	91.366	23.743	-42.507	-.110	.013
2000	14.893	104.626	92.009	25.233	-42.428	2.118	-.231

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
629.81 K, boiling point of Hg; ΔH° = 14.151 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 14.886 + 0.010\times10^{-3}T - 0.429\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.886\times10^{-3}T + 0.005\times10^{-6}T^2 + 0.429\times10^{2}T^{-1} - 4.583$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -19.248 - 9.478\times10^{-3}T + 0.004\times10^{-6}T^2 + 74.300T^{-1}$

$\Delta Gf^\circ = -19.248 + 9.478\times10^{-3}T\ln T - 0.004\times10^{-6}T^2 + 37.150T^{-1} - 85.052\times10^{-3}T$

332.6-629.81 K: $\Delta Hf^\circ = -29.248 - 0.317\times10^{-3}T - 0.151\times10^{-6}T^2 + 42.900T^{-1}$

$\Delta Gf^\circ = -29.248 + 0.317\times10^{-3}T\ln T + 0.151\times10^{-6}T^2 + 21.450T^{-1} - 1.696\times10^{-3}T$

629.81-2000 K: $\Delta Hf^\circ = -44.211 + 0.988\times10^{-3}T - 0.050\times10^{-6}T^2 + 11.500T^{-1}$

$\Delta Gf^\circ = -44.211 - 0.988\times10^{-3}T\ln T + 0.050\times10^{-6}T^2 + 5.750T^{-1} + 30.576\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Vasil'ev (247) and JANAF (60). Other data from JANAF (60).

HgCl(g)

Mercury Monochloride (ideal gas)

[Formation: $Hg(l,g) + 0.5Cl_2(g) = HgCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.705	62.105	62.105	0	18.750	13.586	-9.959
300	8.709	62.159	62.106	.016	18.747	13.554	-9.874
400	8.849	64.685	62.447	.895	18.550	11.854	-6.477
500	8.928	66.669	63.101	1.784	18.360	10.202	-4.459
600	8.981	68.302	63.835	2.680	18.173	8.588	-3.128
629.81	8.993	68.738	64.057	2.948	18.117	8.115	-2.816
629.81	8.993	68.738	64.057	2.948	3.966	8.115	-2.816
700	9.021	69.690	64.576	3.580	3.941	8.579	-2.678
800	9.054	70.896	65.291	4.484	3.906	9.244	-2.525
900	9.083	71.964	65.975	5.390	3.869	9.913	-2.407
1000	9.109	72.923	66.623	6.300	3.836	10.586	-2.313
1100	9.133	73.792	67.236	7.212	3.802	11.262	-2.237
1200	9.157	74.588	67.815	8.127	3.770	11.942	-2.175
1300	9.179	75.322	68.366	9.043	3.739	12.623	-2.122
1400	9.201	76.003	68.887	9.962	3.709	13.309	-2.078
1500	9.222	76.638	69.382	10.884	3.681	13.996	-2.039
1600	9.243	77.234	69.855	11.807	3.653	14.684	-2.006
1700	9.264	77.795	70.306	12.732	3.626	15.374	-1.976
1800	9.285	78.325	70.736	13.660	3.603	16.067	-1.951
1900	9.305	78.828	71.150	14.589	3.579	16.760	-1.928
2000	9.325	79.305	71.545	15.521	3.556	17.457	-1.908

Phase change: 629.81 K, boiling point of Hg; ΔH° = 14.151 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.925 + 0.206\times10^{-3}T - 0.251\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.925\times10^{-3}T + 0.103\times10^{-6}T^2 + 0.251\times10^{2}T^{-1} - 2.754$

Formation equations (kcal/mol):

298.15-629.81 K: $\Delta Hf^\circ = 19.204 - 1.761\times10^{-3}T - 0.042\times10^{-6}T^2 + 22.350T^{-1}$

$\Delta Gf^\circ = 19.204 + 1.761\times10^{-3}T\ln T + 0.042\times10^{-6}T^2 + 11.175T^{-1} - 29.017\times10^{-3}T$

629.81-2000 K: $\Delta Hf^\circ = 4.241 - 0.456\times10^{-3}T + 0.059\times10^{-6}T^2 - 9.050T^{-1}$

$\Delta Gf^\circ = 4.241 + 0.456\times10^{-3}T\ln T - 0.059\times10^{-6}T^2 - 4.525T^{-1} + 3.255\times10^{-3}T$

Source: Data from JANAF (60) who estimated some molecular constants.

$Hg_2Cl_2(c)$

Dimeric Mercury Monochloride

[Formation: $2Hg(l,g) + Cl_2(g) = Hg_2Cl_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	24.371	46.017	46.017	0	-63.319	-50.334	36.895
300*	24.390	46.168	46.018	.045	-63.313	-50.253	36.609
400	25.340	53.318	46.986	2.533	-62.977	-45.947	25.104
500	26.130	59.060	48.846	5.107	-62.560	-41.737	18.243
600	26.800	63.884	50.959	7.755	-62.079	-37.616	13.702
629.81	26.973	65.188	51.602	8.557	-61.924	-36.401	12.631
629.81	26.973	65.188	51.602	8.557	-90.226	-36.401	12.631
655	27.120	66.249	52.145	9.238	-90.016	-34.252	11.429

*Data above 298 K estimated.

Phase changes: 629.81 K, boiling point of Hg; $\Delta H°$ = 14.151 kcal/mol.
655 K, vapor pressure of decomposition products, Hg(g) and $HgCl_2$, = 1 atm.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-655 K: $Cp° = 23.278 + 6.196\times10^{-3}T - 0.671\times10^{5}T^{-2}$

$H°- H°_{298} = 23.278\times10^{-3}T + 3.098\times10^{-6}T^{2} + 0.671\times10^{2}T^{-1} - 7.441$

Formation equations (kcal/mol):

298.15-629.81 K: $\Delta Hf° = -64.343 + 1.905\times10^{-3}T + 2.808\times10^{-6}T^{2} + 61.600T^{-1}$

$\Delta Gf° = -64.343 - 1.905\times10^{-3}T\ln T - 2.808\times10^{-6}T^{2} + 30.800T^{-1} + 58.333\times10^{-3}T$

629.81-655 K: $\Delta Hf° = -94.269 + 4.515\times10^{-3}T + 3.010\times10^{-6}T^{2} - 1.200T^{-1}$

$\Delta Gf° = -94.269 - 4.515\times10^{-3}T\ln T - 3.010\times10^{-6}T^{2} - 0.600T^{-1} + 122.878\times10^{-3}T$

Source: Data from JANAF (60) who estimated data above 298 K.

$HgCl_2$(c,l,g)

Mercury Dichloride

[Formation: $Hg(l,g) + Cl_2(g) = HgCl_2(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	16.620	34.930	34.930	0	-53.600	-42.718	31.312
300	16.640	35.030	34.930	.031	-53.596	-42.649	31.069
400	18.270	40.040	35.603	1.775	-53.343	-39.035	21.328
428	18.730	41.300	35.940	2.295	-53.243	-38.040	19.424
428	16.230	41.480	35.940	2.370	-53.168	-38.040	19.424
500	19.880	44.280	36.940	3.670	-52.953	-35.509	15.521
553.7	22.610	46.440	37.753	4.810	-52.627	-33.650	13.282
553.7	28.160	54.550	37.753	9.300	-48.137	-33.650	13.282
575	28.160	55.610	38.392	9.900	-47.861	-33.096	12.579
575	14.592	79.827	38.392	23.825	-33.936	-33.096	12.579
600	14.621	80.450	40.133	24.190	-33.951	-33.061	12.042
629.81	14.643	81.159	42.059	24.626	-33.969	-33.014	11.456
629.81	14.643	81.159	42.059	24.626	-48.120	-33.014	11.456
700	14.694	82.710	46.059	25.656	-48.055	-31.333	9.783
800	14.742	84.675	50.765	27.128	-47.966	-28.952	7.909
900	14.776	86.414	54.632	28.604	-47.877	-26.579	6.454
1000	14.800	87.972	57.889	30.083	-47.789	-24.219	5.293
1100	14.818	89.383	60.688	31.564	-47.702	-21.866	4.344
1200	14.831	90.673	63.135	33.046	-47.617	-19.521	3.555
1300	14.842	91.861	65.299	34.530	-47.531	-17.184	2.889
1400	14.851	92.961	67.236	36.015	-47.447	-14.851	2.318
1500	14.858	93.986	68.986	37.500	-47.365	-12.528	1.825
1600	14.863	94.945	70.579	38.986	-47.284	-10.207	1.394
1700	14.868	95.846	72.038	40.473	-47.203	-7.890	1.014
1800	14.872	96.696	73.385	41.960	-47.123	-5.581	.678
1900	14.875	97.500	74.633	43.447	-47.045	-3.273	.376
2000	14.878	98.263	75.796	44.935	-46.969	-.971	.106

Phase changes: 428 K, α - β transition point of $HgCl_2$; ΔH° = 0.075 kcal/mol.
553.7 K, melting point of $HgCl_2$; ΔH° = 4.490 kcal/mol.
575 K, boiling point of $HgCl_2$; ΔH° = 13.925 kcal/mol.
629.81 K, boiling point of Hg; ΔH° = 14.151 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-428 K: $Cp^\circ = 9.003 + 21.658\times10^{-3}T + 1.031\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 9.003\times10^{-3}T + 10.829\times10^{-6}T^2 - 1.031\times10^{2}T^{-1} - 3.301$

428-553.7 K: $Cp^\circ = -4.825 + 49.754\times10^{-3}T - 0.437\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = -4.825\times10^{-3}T + 24.877\times10^{-6}T^2 + 0.437\times10^{2}T^{-1} - 0.224$

553.7-575 K: $Cp^\circ = 28.160$

$H^\circ - H^\circ_{298} = 28.160\times10^{-3}T - 6.292$

575-2000 K: $Cp^\circ = 14.904 - 1.032\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.904\times10^{-3}T + 1.032\times10^{2}T^{-1} + 15.076$

$HgCl_2$(c,l,g) - Continued

Formation equations (kcal/mol):

298.15-428 K: $\Delta Hf^\circ = -52.258 - 6.097\times10^{-3}T + 10.640\times10^{-6}T^2 - 140.000T^{-1}$

$\Delta Gf^\circ = -52.258 + 6.097\times10^{-3}T\ln T - 10.640\times10^{-6}T^2 - 70.000T^{-1} + 1.222\times10^{-3}T$

428-553.7 K: $\Delta Hf^\circ = -49.181 - 19.925\times10^{-3}T + 24.688\times10^{-6}T^2 + 6.800T-1$

$\Delta Gf^\circ = -49.181 + 19.925\times10^{-3}T\ln T - 24.688\times10^{-6}T^2 + 3.400T^{-1} - 84.141\times10^{-3}T$

553.7-575 K: $\Delta Hf^\circ = -55.249 + 13.060\times10^{-3}T - 0.189\times10^{-6}T^2 - 36.900T-1$

$\Delta Gf^\circ = -55.249 - 13.060\times10^{-3}T\ln T + 0.189\times10^{-6}T^2 - 18.450T^{-1} + 121.469\times10^{-3}T$

575-629.81 K: $\Delta Hf^\circ = -33.882 - 0.196\times10^{-3}T - 0.189\times10^{-6}T^2 + 66.300T^{-1}$

$\Delta Gf^\circ = -33.882 + 0.196\times10^{-3}T\ln T + 0.189\times10^{-6}T^2 + 33.150T^{-1} - 0.082\times10^{-3}T$

629.81-2000 K: $\Delta Hf^\circ = -48.845 + 1.109\times10^{-3}T - 0.088\times10^{-6}T^2 + 34.900T^{-1}$

$\Delta Gf^\circ = -48.845 - 1.109\times10^{-3}T\ln T + 0.088\times10^{-6}T^2 + 17.450T^{-1} + 32.190\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (253). Data 298 K to 575 K from Cubicciotti (51). Data for gas from JANAF (60).

$HgCl_2(g)$

Mercury Dichloride (ideal gas)

[Formation: $Hg(l,g) + Cl_2(g) = HgCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	13.889	70.433	70.433	0	-33.745	-33.448	24.518
300	13.900	70.519	70.433	.026	-33.746	-33.445	24.365
400	14.299	74.579	70.984	1.438	-33.825	-33.333	18.212
500	14.504	77.794	72.036	2.879	-33.889	-33.202	14.512
600	14.621	80.450	73.223	4.336	-33.950	-33.060	12.042
629.81	14.643	81.159	73.582	4.772	-33.968	-33.013	11.456
629.81	14.643	81.159	73.582	4.772	-48.119	-33.013	11.456
700	14.694	82.710	74.421	5.802	-48.054	-31.332	9.782
800	14.742	84.675	75.583	7.274	-47.965	-28.951	7.909
900	14.776	86.414	76.692	8.750	-47.876	-26.578	6.454
1000	14.800	87.972	77.743	10.229	-47.788	-24.218	5.293
1100	14.818	89.383	78.738	11.710	-47.701	-21.865	4.344
1200	14.831	90.673	79.680	13.192	-47.616	-19.520	3.555
1300	14.842	91.861	80.572	14.676	-47.530	-17.183	2.889
1400	14.851	92.961	81.417	16.161	-47.446	-14.850	2.318
1500	14.858	93.986	82.222	17.646	-47.364	-12.527	1.825
1600	14.863	94.945	82.988	19.132	-47.283	-10.206	1.394
1700	14.868	95.846	83.717	20.619	-47.202	-7.889	1.014
1800	14.872	96.696	84.415	22.106	-47.122	-5.580	.677
1900	14.875	97.500	85.083	23.593	-47.044	-3.272	.376
2000	14.878	98.263	85.723	25.081	-46.968	-.970	.106

Phase change: 629.81 K, boiling point of Hg; ΔH° = 14.151 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 14.821 + 0.052\times10^{-3}T - 0.842\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.821\times10^{-3}T + 0.026\times10^{-6}T^2 + 0.842\times10^{2}T^{-1} - 4.704$

Formation equations (kcal/mol):

298.15-629.81 K: $\Delta Hf^\circ = -33.806 - 0.279\times10^{-3}T - 0.163\times10^{-6}T^2 + 47.300T^{-1}$

$\Delta Gf^\circ = -33.806 + 0.279\times10^{-3}T\ln T + 0.163\times10^{-6}T^2 + 23.650T^{-1} - 0.703\times10^{-3}T$

629.81-2000 K: $\Delta Hf^\circ = -48.769 + 1.026\times10^{-3}T - 0.062\times10^{-6}T^2 + 15.900T^{-1}$

$\Delta Gf^\circ = -48.769 - 1.026\times10^{-3}T\ln T + 0.062\times10^{-6}T^2 + 7.950T^{-1} + 31.570\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Wagman (253) and Cubicciotti (51). Other data from JANAF (60).

$HgF(g)$

Mercury Monofluoride (ideal gas)

[Formation: $Hg(l,g) + 0.5F_2(g) = HgF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH_f°	ΔG_f°	
298.15	8.282	59.338	59.338	0	0.700	-4.362	3.197
300	8.289	59.389	59.339	.015	.696	-4.393	3.200
400	8.570	61.816	59.666	.860	.496	-6.057	3.310
500	8.731	63.747	60.297	1.725	.306	-7.674	3.354
600	8.834	65.349	61.009	2.604	.122	-9.254	3.371
629.81	8.855	65.778	61.225	2.868	.067	-9.716	3.372
629.81	8.855	65.778	61.225	2.868	-14.084	-9.716	3.372
700	8.905	66.716	61.729	3.491	-14.108	-9.227	2.881
800	8.958	67.909	62.429	4.384	-14.142	-8.529	2.330
900	9.001	68.967	63.098	5.282	-14.177	-7.824	1.900
1000	9.036	69.917	63.733	6.184	-14.212	-7.117	1.556
1100	9.067	70.780	64.335	7.090	-14.246	-6.406	1.273
1200	9.095	71.570	64.905	7.998	-14.280	-5.691	1.037
1300	9.121	72.299	65.446	8.909	-14.313	-4.974	.836
1400	9.145	72.976	65.960	9.822	-14.347	-4.254	.664
1500	9.168	73.607	66.448	10.738	-14.380	-3.532	.515
1600	9.189	74.200	66.916	11.655	-14.413	-2.809	.384
1700	9.210	74.758	67.361	12.575	-14.444	-2.084	.268
1800	9.231	75.285	67.787	13.497	-14.474	-1.355	.165
1900	9.251	75.784	68.194	14.421	-14.503	-.623	.072
2000	9.270	76.259	68.585	15.348	-14.531	.108	-.012

Phase change: 629.81 K, boiling point of Hg; $\Delta H^\circ = 14.151$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 8.845 + 0.234\times10^{-3}T - 0.563\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.845\times10^{-3}T + 0.117\times10^{-6}T^2 + 0.563\times10^{2}T^{-1} - 2.836$

Formation equations (kcal/mol):

298.15-629.81 K: $\Delta H_f^\circ = 1.082 - 1.682\times10^{-3}T - 0.071\times10^{-6}T^2 + 37.450T^{-1}$

$\Delta G_f^\circ = 1.082 + 1.682\times10^{-3}T\ln T + 0.071\times10^{-6}T^2 + 18.725T^{-1} - 28.074\times10^{-3}T$

629.81-2000 K: $\Delta H_f^\circ = -13.881 - 0.377\times10^{-3}T + 0.030\times10^{-6}T^2 + 6.050T^{-1}$

$\Delta G_f^\circ = -13.881 + 0.377\times10^{-3}T\ln T - 0.030\times10^{-6}T^2 + 3.025T^{-1} + 4.199\times10^{-3}T$

Source: Data from JANAF (60) who estimated some molecular constants.

$Hg_2F_2(c)$

Dimeric Mercury Monofluoride

[Formation: $2Hg(l,g) + F_2(g) = Hg_2F_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15*	24.000	38.400	38.400	0	-116.000	-102.189	74.905
300	24.020	38.549	38.402	.044	-115.994	-102.103	74.381
400	25.020	45.599	39.354	2.498	-115.631	-97.523	53.284
500	25.910	51.280	41.190	5.045	-115.192	-93.047	40.670
600	26.690	56.075	43.282	7.676	-114.689	-88.666	32.296
629.81	26.893	57.374	43.918	8.475	-114.527	-87.373	30.319
629.81	26.893	57.374	43.918	8.475	-142.829	-87.373	30.319
700	27.370	60.241	45.412	10.380	-142.217	-81.223	25.358
800	27.950	63.935	47.501	13.147	-141.306	-72.572	19.826
900	28.430	67.255	49.515	15.966	-140.352	-64.036	15.550
949	28.640	68.768	50.471	17.364	-139.871	-59.894	13.793

*Data estimated except Gibbs energy of formation at 298 K.

Phase changes: 629.81 K, boiling point of Hg; $\Delta H°$ = 14.151 kcal/mol.
949 K, vapor pressure of decomposition products, Hg(g) and $HgF_2(g)$, = 1 atm.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-949 K: $Cp° = 23.453 + 5.762\times10^{-3}T - 1.042\times10^{5}T^{-2}$

$H°- H°_{298} = 23.453\times10^{-3}T + 2.881\times10^{-6}T^2 + 1.042\times10^{2}T^{-1} - 7.598$

Formation equations (kcal/mol):

298.15-629.81 K: $\Delta Hf° = -117.161 + 2.399\times10^{-3}T + 2.505\times10^{-6}T^2 + 66.500T^{-1}$

$\Delta Gf° = -117.161 - 2.399\times10^{-3}T\ln T - 2.505\times10^{-6}T^2 + 33.250T^{-1} + 64.258\times10^{-3}T$

629.81-949 K: $\Delta Hf° = -147.087 + 5.009\times10^{-3}T + 2.707\times10^{-6}T^2 + 3.700T^{-1}$

$\Delta Gf° = -147.087 - 5.009\times10^{-3}T\ln T - 2.707\times10^{-6}T^2 + 1.850T^{-1} + 128.804\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except Gibbs energy of formation at 298 K.

$HgF_2(c,l,g)$

Mercury Difluoride

[Formation: $Hg(l,g) + F_2(g) = HgF_2(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	17.891	27.800	27.800	0	-101.000	-89.437	65.558
300	17.900	27.911	27.801	.033	-100.993	-89.365	65.102
400	18.400	33.128	28.508	1.848	-100.608	-85.546	46.739
500	18.900	37.288	29.862	3.713	-100.199	-81.827	35.766
600	19.400	40.778	31.398	5.628	-99.763	-78.194	28.482
629.81	19.549	41.722	31.865	6.209	-99.627	-77.124	26.762
629.81	19.549	41.722	31.865	6.209	-113.778	-77.124	26.762
700	19.900	43.806	32.959	7.593	-113.338	-73.061	22.811
800	20.400	46.496	34.486	9.608	-112.682	-67.353	18.400
900	20.900	48.927	35.957	11.673	-111.985	-61.726	14.989
918	20.990	49.340	36.214	12.050	-111.855	-60.721	14.456
918	24.400	55.331	36.214	17.550	-106.355	-60.721	14.456
920	24.400	55.383	36.254	17.599	-106.334	-60.620	14.400
920	14.615	79.291	36.254	39.594	-84.339	-60.620	14.400
1000	14.659	80.512	39.747	40.765	-84.270	-58.563	12.799
1100	14.701	81.911	43.517	42.233	-84.185	-55.996	11.125
1200	14.732	83.192	46.771	43.705	-84.101	-53.437	9.732
1300	14.757	84.372	49.619	45.179	-84.018	-50.885	8.554
1400	14.777	85.466	52.140	46.656	-83.938	-48.339	7.546
1500	14.793	86.486	54.396	48.135	-83.859	-45.799	6.673
1600	14.807	87.441	56.432	49.615	-83.782	-43.264	5.909
1700	14.818	88.339	58.283	51.096	-83.706	-40.733	5.237
1800	14.827	89.187	59.977	52.578	-83.632	-38.209	4.639
1900	14.835	89.989	61.536	54.061	-83.559	-35.687	4.105
2000	14.842	90.750	62.978	55.545	-83.489	-33.169	3.624

*Data estimated except temperatures of fusion and boiling.

Phase changes: 629.81 K, boiling point of Hg; ΔH° = 14.151 kcal/mol.
918 K, melting point of HgF_2; ΔH° = 5.500 kcal/mol.
920 K, boiling point of HgF_2; ΔH° = 21.995 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-918 K: $Cp^\circ = 16.398 + 5.002\times10^{-3}T + 0.001\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 16.398\times10^{-3}T + 2.501\times10^{-6}T^2 - 0.001\times10^{2}T^{-1} - 5.111$

918-920 K: $Cp^\circ = 24.440$

$H^\circ - H^\circ_{298} = 24.440\times10^{-3}T - 4.886$

920-2000 K: $Cp^\circ = 14.913 - 0.006\times10^{-3}T - 2.469\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.913\times10^{-3}T - 0.003\times10^{-6}T^2 + 2.469\times10^{2}T^{-1} + 25.608$

HgF_2(c,l,g) - Continued

Formation equations (kcal/mol):

298.15-629.81 K: $\Delta Hf^\circ = -101.448 + 1.617\times10^{-3}T + 2.226\times10^{-6}T^2 - 69.200T^{-1}$

$\Delta Gf^\circ = -101.448 - 1.617\times10^{-3}T\ln T - 2.226\times10^{-6}T^2 - 34.600T^{-1} + 50.551\times10^{-3}T$

629.81-918 K: $\Delta Hf^\circ = -116.411 + 2.922\times10^{-3}T + 2.327\times10^{-6}T^2 - 100.600T^{-1}$

$\Delta Gf^\circ = -116.411 - 2.922\times10^{-3}T\ln T - 2.327\times10^{-6}T^2 - 50.300T^{-1} + 82.824\times10^{-3}T$

918-920 K: $\Delta Hf^\circ = -116.186 + 10.964\times10^{-3}T - 0.174\times10^{-6}T^2 - 100.500T^{-1}$

$\Delta Gf^\circ = -116.186 - 10.964\times10^{-3}T\ln T + 0.174\times10^{-6}T^2 - 50.250T^{-1} + 135.147\times10^{-3}T$

920-2000 K: $\Delta Hf^\circ = -85.692 + 1.437\times10^{-3}T - 0.177\times10^{-6}T^2 + 146.400T^{-1}$

$\Delta Gf^\circ = -85.692 - 1.437\times10^{-3}T\ln T + 0.177\times10^{-6}T^2 + 73.200T^{-1} + 36.837\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except temperatures of fusion and boiling.

$HgF_2(g)$

Mercury Difluoride (ideal gas)

[Formation: $Hg(l,g) + F_2(g) = HgF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	12.899	63.545	63.545	0	-70.190	-69.284	50.786
300	12.916	63.624	63.545	.024	-70.192	-69.278	50.468
400	13.614	67.445	64.060	1.354	-70.292	-68.956	37.676
500	14.018	70.530	65.056	2.737	-70.365	-68.614	29.991
600	14.263	73.110	66.190	4.152	-70.429	-68.259	24.863
629.81	14.310	73.803	66.534	4.578	-70.447	-68.149	23.648
629.81	14.310	73.803	66.534	4.578	-84.598	-68.149	23.648
700	14.422	75.321	67.340	5.587	-84.534	-66.318	20.705
800	14.529	77.254	68.460	7.035	-84.445	-63.723	17.408
900	14.604	78.970	69.534	8.492	-84.356	-61.136	14.846
1000	14.659	80.512	70.557	9.955	-84.270	-58.563	12.799
1100	14.701	81.911	71.526	11.423	-84.185	-55.996	11.125
1200	14.732	83.192	72.446	12.895	-84.101	-53.437	9.732
1300	14.757	84.372	73.319	14.369	-84.018	-50.885	8.554
1400	14.777	85.466	74.147	15.846	-83.938	-48.339	7.546
1500	14.793	86.486	74.936	17.325	-83.859	-45.799	6.673
1600	14.807	87.441	75.688	18.805	-83.782	-43.264	5.909
1700	14.818	88.339	76.406	20.286	-83.706	-40.733	5.237
1800	14.827	89.187	77.094	21.768	-83.632	-38.209	4.639
1900	14.835	89.989	77.752	23.251	-83.559	-35.687	4.105
2000	14.842	90.750	78.382	24.735	-83.489	-33.169	3.624

*All data estimated.

Phase change: 629.81 K, boiling point of Hg; ΔH° = 14.151 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 14.542 + 0.224\times10^{-3}T - 1.520\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.542\times10^{-3}T + 0.112\times10^{-6}T^2 + 1.520\times10^{2}T^{-1} - 4.855$

Formation equations (kcal/mol):

298.15-629.81 K: $\Delta Hf^\circ = -70.382 - 0.239\times10^{-3}T - 0.163\times10^{-6}T^2 + 82.900T^{-1}$

$\Delta Gf^\circ = -70.382 + 0.239\times10^{-3}T\ln T + 0.163\times10^{-6}T^2 + 41.450T^{-1} + 1.806\times10^{-3}T$

629.81-2000 K: $\Delta Hf^\circ = -85.345 + 1.066\times10^{-3}T - 0.062\times10^{-6}T^2 + 51.500T^{-1}$

$\Delta Gf^\circ = -85.345 - 1.066\times10^{-3}T\ln T + 0.062\times10^{-6}T^2 + 25.750T^{-1} + 34.079\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

HgI(g)

Mercury Monoiodide (ideal gas)

[Formation: $Hg(l,g) + 0.5I_2(c,l,g) = HgI(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	9.055	67.068	67.068	0	31.900	21.450	-15.723
300	9.056	67.124	67.068	.017	31.893	21.386	-15.579
386.8	9.128	69.435	67.350	.806	31.504	18.396	-10.394
386.8	9.128	69.435	67.350	.806	29.650	18.396	-10.394
400	9.139	69.741	67.424	.927	29.556	18.014	-9.842
458.4	9.179	70.989	67.801	1.462	29.147	16.358	-7.799
458.4	9.179	70.989	67.801	1.462	24.136	16.358	-7.799
500	9.208	71.788	68.100	1.844	24.062	15.656	-6.843
600	9.272	73.473	68.860	2.768	23.889	13.989	-5.096
629.81	9.290	73.923	69.089	3.045	23.838	13.501	-4.685
629.81	9.290	73.923	69.089	3.045	9.687	13.501	-4.685
700	9.333	74.907	69.624	3.698	9.677	13.927	-4.348
800	9.393	76.157	70.363	4.635	9.667	14.536	-3.971
900	9.452	77.266	71.069	5.577	9.660	15.145	-3.678
1000	9.511	78.265	71.740	6.525	9.658	15.755	-3.443
1100	9.569	79.175	72.376	7.479	9.662	16.362	-3.251
1200	9.627	80.010	72.978	8.439	9.670	16.972	-3.091
1300	9.685	80.783	73.548	9.405	9.686	17.580	-2.955
1400	9.743	81.503	74.092	10.376	9.704	18.188	-2.839
1500	9.801	82.177	74.608	11.353	9.727	18.791	-2.738
1600	9.858	82.811	75.101	12.336	9.756	19.396	-2.649
1700	9.916	83.410	75.572	13.325	9.790	19.998	-2.571
1800	9.973	83.979	76.024	14.319	9.830	20.596	-2.501
1900	10.031	84.520	76.457	15.320	9.874	21.194	-2.438
2000	10.088	85.036	76.873	16.326	9.923	21.789	-2.381

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
629.81 K, boiling point of Hg; ΔH° = 14.151 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.942 + 0.574\times10^{-3}T - 0.052\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.942\times10^{-3}T + 0.287\times10^{-6}T^2 + 0.052\times10^{2}T^{-1} - 2.709$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = 32.951 - 3.769\times10^{-3}T - 0.560\times10^{-6}T^2 + 36.600T^{-1}$

$\Delta Gf^\circ = 32.951 + 3.769\times10^{-3}T\ln T + 0.560\times10^{-6}T^2 + 18.300T^{-1} - 60.424\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = 32.223 - 6.971\times10^{-3}T + 0.186\times10^{-6}T^2 + 36.600T^{-1}$

$\Delta Gf^\circ = 32.223 + 6.971\times10^{-3}T\ln T - 0.186\times10^{-6}T^2 + 18.300T^{-1} - 77.331\times10^{-3}T$

458.4-629.81 K: $\Delta Hf^\circ = 24.867 - 1.801\times10^{-3}T + 0.152\times10^{-6}T^2 + 28.950T^{-1}$

$\Delta Gf^\circ = 24.867 + 1.801\times10^{-3}T\ln T - 0.152\times10^{-6}T^2 + 14.475T^{-1} - 29.600\times10^{-3}T$

629.81-2000 K: $\Delta Hf^\circ = 9.904 - 0.497\times10^{-3}T + 0.253\times10^{-6}T^2 - 2.450T^{-1}$

$\Delta Gf^\circ = 9.904 + 0.497\times10^{-3}T\ln T - 0.253\times10^{-6}T^2 - 1.225T^{-1} + 2.673\times10^{-3}T$

Source: Data from JANAF (60) who estimated some molecular constants.

Hg_2I_2(c,l)

Dimeric Mercury Monoiodide

[Formation: $2Hg(l,g) + I_2(c,l,g) = Hg_2I_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	25.300	57.670	57.670	0	-28.462	-26.563	19.471
300	25.323	57.827	57.670	.047	-28.463	-26.551	19.342
386.8	26.249	64.383	58.469	2.288	-28.579	-25.984	14.681
386.8	26.249	64.383	58.469	2.288	-32.288	-25.984	14.681
400	26.390	65.266	58.678	2.635	-32.369	-25.767	14.078
458.4	26.846	68.897	59.753	4.191	-32.700	-24.778	11.813
458.4	26.846	68.897	59.753	4.191	-42.721	-24.778	11.813
500	27.170	71.243	60.613	5.315	-42.511	-23.157	10.122
563	27.530	74.470	61.948	7.050	-42.159	-20.719	8.043
563	32.600	86.015	61.948	13.550	-35.659	-20.719	8.043
600	32.600	88.090	63.498	14.755	-35.266	-19.751	7.194
629.81	32.600	89.671	64.700	15.727	-34.948	-18.984	6.588
629.81	32.600	89.671	64.700	15.727	-63.250	-18.984	6.588
630	32.600	89.681	64.708	15.733	-63.247	-18.970	6.581

*Entropy at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
563 K, melting point of Hg_2I_2; $\Delta H°$ = 6.500 kcal/mol.
629.81 K, boiling point of Hg; $\Delta H°$ = 14.151 kcal/mol.
630 K, vapor pressure of decomposition products, Hg(g) and HgI_2(g), = 1 atm.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-563 K: $Cp° = 23.530 + 7.890\times10^{-3}T - 0.518\times10^{5}T^{-2}$

$H°- H°_{298} = 23.530\times10^{-3}T + 3.945\times10^{-6}T^2 + 0.518\times10^{2}T^{-1} - 7.540$

563-630 K: $Cp° = 32.600$

$H°- H°_{298} = 32.600\times10^{-3}T - 4.804$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -28.482 - 1.893\times10^{-3}T + 2.251\times10^{-6}T^2 + 114.600T^{-1}$

$\Delta Gf° = -28.482 + 1.893\times10^{-3}T\ln T - 2.251\times10^{-6}T^2 + 57.300T^{-1} - 4.324\times10^{-3}T$

386.8-458.4 K: $\Delta Hf° = -29.937 - 8.297\times10^{-3}T + 3.743\times10^{-6}T^2 + 114.600T^{-1}$

$\Delta Gf° = -29.937 + 8.297\times10^{-3}T\ln T - 3.743\times10^{-6}T^2 + 57.300T^{-1} - 38.139\times10^{-3}T$

458.4-563 K: $\Delta Hf° = -44.650 + 2.043\times10^{-3}T + 3.675\times10^{-6}T^2 + 99.300T^{-1}$

$\Delta Gf° = -44.650 - 2.043\times10^{-3}T\ln T - 3.675\times10^{-6}T^2 + 49.650T^{-1} + 57.324\times10^{-3}T$

563-629.81 K: $\Delta Hf° = -41.914 + 11.113\times10^{-3}T - 0.270\times10^{-6}T^2 + 47.500T^{-1}$

$\Delta Gf° = -41.914 - 11.113\times10^{-3}T\ln T + 0.270\times10^{-6}T^2 + 23.750T^{-1} + 107.768\times10^{-3}T$

629.81-630 K: $\Delta Hf° = -71.841 + 13.723\times10^{-3}T - 0.068\times10^{-6}T^2 - 15.300T^{-1}$

$\Delta Gf° = -71.841 - 13.723\times10^{-3}T\ln T + 0.068\times10^{-6}T^2 - 7.650T^{-1} + 172.313\times10^{-3}T$

Source: Data from JANAF (60) who estimated entropy at 298 K.

$HgI_2(c,l,g)$
Mercury Diiodide
[Formation: $Hg(l,g) + I_2(c,l,g) = HgI_2(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	18.582	43.338	43.338	0	-25.200	-24.437	17.912
300	18.600	43.453	43.340	.034	-25.202	-24.432	17.798
386.8	19.468	48.286	43.926	1.686	-25.332	-24.194	13.670
386.8	19.468	48.286	43.926	1.686	-29.041	-24.194	13.670
400	19.600	48.941	44.081	1.944	-29.125	-24.027	13.128
402	19.600	49.038	44.103	1.984	-29.137	-24.000	13.048
402	20.105	50.531	44.103	2.584	-28.537	-24.000	13.048
458.4	20.105	53.171	45.061	3.718	-28.858	-23.341	11.128
458.4	20.105	53.171	45.061	3.718	-38.879	-23.341	11.128
500	20.105	54.917	45.809	4.554	-38.685	-21.938	9.589
530	20.105	56.088	46.358	5.157	-38.545	-20.937	8.633
530	24.400	64.643	46.358	9.691	-34.011	-20.937	8.633
600	24.400	67.670	48.672	11.399	-33.386	-19.251	7.012
627	24.400	68.744	49.513	12.058	-33.144	-18.618	6.490
627	14.833	91.297	49.513	26.199	-19.003	-18.618	6.490
629.81	14.834	91.363	49.699	26.241	-19.005	-18.616	6.460
629.81	14.834	91.363	49.699	26.241	-33.156	-18.616	6.460
700	14.848	92.928	53.954	27.282	-33.094	-16.996	5.306
800	14.861	94.911	58.951	28.768	-33.006	-14.701	4.016
900	14.870	96.662	63.045	30.255	-32.920	-12.418	3.015
1000	14.877	98.229	66.487	31.742	-32.835	-10.145	2.217
1100	14.882	99.648	69.439	33.230	-32.751	-7.882	1.566
1200	14.885	100.943	72.011	34.718	-32.669	-5.625	1.024
1300	14.888	102.134	74.282	36.207	-32.585	-3.373	.567
1400	14.890	103.238	76.312	37.696	-32.505	-1.128	.176
1500	14.892	104.265	78.142	39.185	-32.426	1.108	-.161
1600	14.894	105.226	79.805	40.674	-32.348	3.343	-.457
1700	14.895	106.129	81.327	42.164	-32.271	5.571	-.716
1800	14.896	106.981	82.729	43.653	-32.195	7.794	-.946
1900	14.897	107.786	84.027	45.143	-32.121	10.015	-1.152
2000	14.898	108.550	85.234	46.633	-32.048	12.232	-1.337

*Entropy at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
402 K, α - β transition point of HgI_2; $\Delta H°$ = 0.600 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
530 K, melting point of HgI_2; $\Delta H°$ = 4.534 kcal/mol.
627 K, boiling point of HgI_2; $\Delta H°$ = 14.141 kcal/mol.
629.81 K, boiling point of Hg; $\Delta H°$ = 14.151 kcal/mol.

HgI_2(c,l,g) - Continued

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-402 K: $Cp^\circ = 15.582 + 10.062\times10^{-3}T$

$H^\circ - H^\circ_{298} = 15.582\times10^{-3}T + 5.031\times10^{-6}T^2 - 5.093$

402-530 K: $Cp^\circ = 20.106$

$H^\circ - H^\circ_{298} = 20.106\times10^{-3}T - 5.499$

530-627 K: $Cp^\circ = 24.400$

$H^\circ - H^\circ_{298} = 24.400\times10^{-3}T - 3.241$

627-2000 K: $Cp^\circ = 14.911 - 0.004\times10^{-3}T - 0.298\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.911\times10^{-3}T - 0.002\times10^{-6}T^2 + 0.298\times10^{2}T^{-1} + 16.803$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -24.547 - 3.568\times10^{-3}T + 3.438\times10^{-6}T^2 + 31.400T^{-1}$

$\Delta Gf^\circ = -24.547 + 3.568\times10^{-3}T\ln T - 3.438\times10^{-6}T^2 + 15.700T^{-1} - 19.110\times10^{-3}T$

386.8-402 K: $\Delta Hf^\circ = -26.002 - 9.972\times10^{-3}T + 4.930\times10^{-6}T^2 + 31.400T^{-1}$

$\Delta Gf^\circ = -26.002 + 9.972\times10^{-3}T\ln T - 4.930\times10^{-6}T^2 + 15.700T^{-1} - 52.926\times10^{-3}T$

402-458.4 K: $\Delta Hf^\circ = -26.408 - 5.448\times10^{-3}T - 0.101\times10^{-6}T^2 + 31.400T^{-1}$

$\Delta Gf^\circ = -26.408 + 5.448\times10^{-3}T\ln T + 0.101\times10^{-6}T^2 + 15.700T^{-1} - 26.811\times10^{-3}T$

458.4-530 K: $\Delta Hf^\circ = -41.121 + 4.892\times10^{-3}T - 0.169\times10^{-6}T^2 + 16.100T^{-1}$

$\Delta Gf^\circ = -41.121 - 4.892\times10^{-3}T\ln T + 0.169\times10^{-6}T^2 + 8.050T^{-1} + 68.652\times10^{-3}T$

530-627 K: $\Delta Hf^\circ = -38.863 + 9.186\times10^{-3}T - 0.169\times10^{-6}T^2 + 16.100T^{-1}$

$\Delta Gf^\circ = -38.863 - 9.186\times10^{-3}T\ln T + 0.169\times10^{-6}T^2 + 8.050T^{-1} + 91.327\times10^{-3}T$

627-629.81 K: $\Delta Gf^\circ = -18.819 - 0.303\times10^{-3}T - 0.171\times10^{-6}T^2 + 45.900T^{-1}$

$\Delta Gf^\circ = -18.819 + 0.303\times10^{-3}T\ln T + 0.171\times10^{-6}T^2 + 22.950T^{-1} - 1.798\times10^{-3}T$

629.81-2000 K: $\Delta Hf^\circ = -33.782 + 1.002\times10^{-3}T - 0.070\times10^{-6}T^2 + 14.500T^{-1}$

$\Delta Gf^\circ = -33.782 - 1.002\times10^{-3}T\ln T + 0.070\times10^{-6}T^2 + 7.250T^{-1} + 30.474\times10^{-3}T$

Source: Data from JANAF (60) who estimated entropy at 298 K.

$HgI_2(g)$
Mercury Diiodide (ideal gas)
[Formation: $Hg(l,g) + I_2(c,l,g) = HgI_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	14.608	80.331	80.331	0	-3.855	-14.121	10.351
300	14.611	80.421	80.331	.027	-3.864	-14.184	10.333
386.8	14.719	84.150	80.787	1.301	-4.373	-17.107	9.665
386.8	14.719	84.150	80.787	1.301	-8.082	-17.107	9.665
400	14.736	84.644	80.906	1.495	-8.229	-17.412	9.513
458.4	14.771	86.656	81.514	2.357	-8.873	-18.706	8.918
458.4	14.771	86.656	81.514	2.357	-18.894	-18.706	8.918
500	14.796	87.940	81.996	2.972	-18.922	-18.686	8.168
600	14.828	90.640	83.217	4.454	-18.986	-18.633	6.787
629.81	14.834	91.359	83.585	4.896	-19.005	-18.613	6.459
629.81	14.834	91.359	83.585	4.896	-33.156	-18.613	6.459
700	14.848	92.928	84.447	5.937	-33.094	-16.996	5.306
800	14.861	94.911	85.632	7.423	-33.006	-14.701	4.016
900	14.870	96.662	86.762	8.910	-32.920	-12.418	3.015
1000	14.877	98.229	87.832	10.397	-32.835	-10.145	2.217
1100	14.882	99.648	88.843	11.885	-32.751	-7.882	1.566
1200	14.885	100.943	89.799	13.373	-32.669	-5.625	1.024
1300	14.888	102.134	90.702	14.862	-32.585	-3.373	.567
1400	14.890	103.238	91.559	16.351	-32.505	-1.128	.176
1500	14.892	104.265	92.372	17.840	-32.426	1.108	-.161
1600	14.894	105.226	93.145	19.329	-32.348	3.343	-.457
1700	14.895	106.129	93.883	20.819	-32.271	5.571	-.716
1800	14.896	106.981	94.588	22.308	-32.195	7.794	-.946
1900	14.897	107.786	95.261	23.798	-32.121	10.015	-1.152
2000	14.898	108.550	95.906	25.288	-32.048	12.232	-1.337

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
629.81 K, boiling point of Hg; $\Delta H°$ = 14.151 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 14.900 + 0.002\times10^{-3}T - 0.260\times10^{5}T^{-2}$
$H°- H°_{298} = 14.900\times10^{-3}T + 0.001\times10^{-6}T^2 + 0.260\times10^{2}T^{-1} - 4.530$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -2.639 - 4.250\times10^{-3}T - 1.592\times10^{-6}T^2 + 57.400T^{-1}$
$\Delta Gf° = -2.639 + 4.250\times10^{-3}T\ln T + 1.592\times10^{-6}T^2 + 28.700T^{-1} - 63.524\times10^{-3}T$
386.8-458.4 K: $\Delta Hf° = -4.094 - 10.654\times10^{-3}T - 0.100\times10^{-6}T^2 + 57.400T^{-1}$
$\Delta Gf° = -4.094 + 10.654\times10^{-3}T\ln T + 0.100\times10^{-6}T^2 + 28.700T^{-1} - 97.340\times10^{-3}T$
458.4-629.81 K: $\Delta Hf° = -18.807 - 0.314\times10^{-3}T - 0.168\times10^{-6}T^2 + 42.100T^{-1}$
$\Delta Gf° = -18.807 + 0.314\times10^{-3}T\ln T + 0.168\times10^{-6}T^2 + 21.050T^{-1} - 1.877\times10^{-3}T$
629.81-2000 K: $\Delta Hf° = -33.770 + 0.991\times10^{-3}T - 0.067\times10^{-6}T^2 + 10.700T^{-1}$
$\Delta Gf° = -33.770 - 0.991\times10^{-3}T\ln T + 0.067\times10^{-6}T^2 + 5.350T^{-1} + 30.396\times10^{-3}T$

Source: Data from JANAF (60).

$HoBr_3(c,l)$

Holmium Tribromide

[Formation: $Ho(c) + 1.5Br_2(l,g) = HoBr_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	23.600	46.400	46.400	0	-201.000	-193.219	141.631
300	23.626	46.546	46.400	.044	-201.017	-193.169	140.722
332.6	23.920	48.998	46.536	.819	-201.337	-192.300	126.358
332.6	23.920	48.998	46.536	.819	-211.934	-192.300	126.358
400	24.528	53.487	47.340	2.459	-211.624	-188.356	102.912
500	24.932	59.008	49.140	4.934	-211.141	-182.592	79.810
600	25.194	63.578	51.178	7.440	-210.643	-176.931	64.446
700	25.437	67.480	53.234	9.972	-210.126	-171.353	53.498
800	25.714	70.894	55.233	12.529	-209.598	-165.846	45.307
900	26.047	73.941	57.145	15.116	-209.071	-160.408	38.952
1000	26.451	76.706	58.965	17.741	-208.539	-155.032	33.882
1100	26.932	79.248	60.694	20.409	-208.007	-149.713	29.745
1192	27.446	81.432	62.212	22.910	-207.516	-144.850	26.557
1192	34.400	91.474	62.212	34.880	-195.546	-144.850	26.557
1200	34.400	91.704	62.408	35.155	-195.448	-144.510	26.319
1300	34.400	94.457	64.769	38.595	-194.254	-140.316	23.589

*Entropy and heat capacity at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
1192 K, melting point of $HoBr_3$; ΔH° = 11.970 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1192 K: $Cp^\circ = 24.158 + 2.404\times10^{-3}T - 1.131\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 24.158\times10^{-3}T + 1.202\times10^{-6}T^2 + 1.131\times10^{2}T^{-1} - 7.689$

1192-1300 K: $Cp^\circ = 34.400$

$H^\circ - H^\circ_{298} = 34.400\times10^{-3}T - 6.125$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -199.934 - 6.319\times10^{-3}T - 0.973\times10^{-6}T^2 + 269.800T^{-1}$

$\Delta Gf^\circ = -199.934 + 6.319\times10^{-3}T\ln T + 0.973\times10^{-6}T^2 + 134.900T^{-1} - 15.290\times10^{-3}T$

332.6-1192 K: $\Delta Hf^\circ = -214.935 + 7.422\times10^{-3}T - 1.206\times10^{-6}T^2 + 222.700T^{-1}$

$\Delta Gf^\circ = -214.935 - 7.422\times10^{-3}T\ln T + 1.206\times10^{-6}T^2 + 111.350T^{-1} + 109.743\times10^{-3}T$

1192-1300 K: $\Delta Hf^\circ = -213.371 + 17.664\times10^{-3}T - 2.408\times10^{-6}T^2 + 109.600T^{-1}$

$\Delta Gf^\circ = -213.371 - 17.664\times10^{-3}T\ln T + 2.408\times10^{-6}T^2 + 54.800T^{-1} + 179.586\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Kim (122). Entropy and heat capacity at 298 K estimated. High-temperature data based on Dworkin (69).

$HoBr_3(g)$

Holmium Tribromide (ideal gas)

[Formation: $Ho(c,l) + 1.5Br_2(l,g) = HoBr_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.089	96.555	96.555	0	-131.100	-138.272	101.355
300	19.097	96.673	96.556	.035	-131.126	-138.316	100.762
332.6	19.203	98.648	96.666	.659	-131.597	-139.074	91.384
332.6	19.203	98.648	96.666	.659	-142.194	-139.074	91.384
400	19.422	102.218	97.308	1.964	-142.219	-138.444	75.641
500	19.580	106.571	98.743	3.914	-142.262	-137.494	60.098
600	19.669	110.149	100.354	5.877	-142.307	-136.536	49.733
700	19.726	113.185	101.975	7.847	-142.351	-135.572	42.327
800	19.770	115.822	103.545	9.822	-142.406	-134.596	36.769
900	19.812	118.153	105.041	11.801	-142.486	-133.614	32.445
1000	19.855	120.243	106.459	13.784	-142.596	-132.626	28.985
1100	19.904	122.138	107.800	15.772	-142.744	-131.629	26.152
1200	19.958	123.872	109.068	17.765	-142.938	-130.602	23.785
1300	20.017	125.471	110.268	19.764	-143.185	-129.565	21.782
1400	20.078	126.957	111.408	21.769	-143.494	-128.501	20.060
1500	20.140	128.344	112.491	23.780	-143.873	-127.417	18.564
1600	20.202	129.646	113.523	25.797	-144.330	-126.314	17.254
1700	20.262	130.873	114.508	27.820	-144.871	-125.169	16.091
1701	20.263	130.885	114.518	27.840	-144.877	-125.170	16.082
1701	20.263	130.885	114.518	27.840	-145.998	-125.170	16.082
1743	20.287	131.379	114.918	28.692	-146.001	-124.643	15.628
1743	20.287	131.379	114.918	28.692	-148.912	-124.643	15.628
1800	20.319	132.033	115.450	29.849	-149.133	-123.842	15.036
1900	20.372	133.133	116.352	31.884	-149.516	-122.438	14.083
2000	20.420	134.179	117.217	33.923	-149.898	-121.003	13.222

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.
1701 K, α - β transition point of Ho; $\Delta H° = 1.121$ kcal/mol.
1743 K, melting point of Ho; $\Delta H° = 2.911$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.549 + 0.406\times10^{-3}T - 0.517\times10^{5}T^{-2}$

$H°- H°_{298} = 19.549\times10^{-3}T + 0.203\times10^{-6}T^2 + 0.517\times10^{2}T^{-1} - 6.020$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -128.365 - 10.929\times10^{-3}T - 1.972\times10^{-6}T^2 + 208.400T^{-1}$

$\Delta Gf° = -128.365 + 10.929\times10^{-3}T\ln T + 1.972\times10^{-6}T^2 + 104.200T^{-1} - 97.255\times10^{-3}T$

332.6-1701 K: $\Delta Hf° = -143.366 + 2.813\times10^{-3}T - 2.205\times10^{-6}T^2 + 161.300T^{-1}$

$\Delta Gf° = -143.366 - 2.813\times10^{-3}T\ln T + 2.205\times10^{-6}T^2 + 80.650T^{-1} + 27.778\times10^{-3}T$

1701-1743 K: $\Delta Hf° = -145.408 - 0.546\times10^{-3}T + 0.121\times10^{-6}T^2 + 4.600T^{-1}$

$\Delta Gf° = -145.408 + 0.546\times10^{-3}T\ln T - 0.121\times10^{-6}T^2 + 2.300T^{-1} + 7.973\times10^{-3}T$

1743-2000 K: $\Delta Hf° = -141.696 - 4.346\times10^{-3}T + 0.121\times10^{-6}T^2 + 4.600T^{-1}$

$\Delta Gf° = -141.696 + 4.346\times10^{-3}T\ln T - 0.121\times10^{-6}T^2 + 2.300T^{-1} - 22.518\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

$HoCl_3(c,l)$

Holmium Trichloride

[Formation: $Ho(c) + 1.5Cl_2(g) = HoCl_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	23.000	36.800	36.800	0	-240.300	-222.093	162.797
300	23.040	36.942	36.800	.043	-240.292	-221.980	161.710
400	24.142	43.762	37.722	2.416	-239.822	-215.947	117.987
500	24.348	49.178	39.492	4.843	-239.344	-210.031	91.803
600	24.414	53.622	41.487	7.281	-238.885	-204.213	74.384
700	24.597	57.397	43.497	9.730	-238.429	-198.471	61.965
800	25.006	60.705	45.445	12.208	-237.967	-192.793	52.668
900	25.692	63.687	47.309	14.740	-237.480	-187.172	45.451
993	26.602	66.255	48.964	17.170	-236.987	-182.001	40.056
993	34.300	73.632	48.964	24.495	-229.662	-182.001	40.056
1000	34.300	73.873	49.138	24.735	-229.570	-181.666	39.702
1100	34.300	77.142	51.537	28.165	-228.268	-176.945	35.155
1200	34.300	80.127	53.798	31.595	-227.020	-172.328	31.385
1300	34.300	82.872	55.930	35.025	-225.832	-167.820	28.213

*Entropy and heat capacity at 298 K estimated.

Phase change: 993 K, melting point of $HoCl_3$; $\Delta H° = 7.325$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-993 K: $Cp° = 24.573 + 1.096\times10^{-3}T - 1.691\times10^{5}T^{-2}$

$H°- H°_{298} = 24.573\times10^{-3}T + 0.548\times10^{-6}T^2 + 1.691\times10^{2}T^{-1} - 7.942$

993-1300 K: $Cp° = 34.300$

$H°- H°_{298} = 34.300\times10^{-3}T - 9.565$

Formation equations (kcal/mol):

298.15-993 K: $\Delta Hf° = -243.262 + 7.992\times10^{-3}T - 1.909\times10^{-6}T^2 + 223.350T^{-1}$

$\Delta Gf° = -243.262 - 7.992\times10^{-3}T\ln T + 1.909\times10^{-6}T^2 + 111.675T^{-1} + 114.707\times10^{-3}T$

993-1300 K: $\Delta Hf° = -244.885 + 17.719\times10^{-3}T - 2.457\times10^{-6}T^2 + 54.250T^{-1}$

$\Delta Gf° = -244.885 - 17.719\times10^{-3}T\ln T + 2.457\times10^{-6}T^2 + 27.125T^{-1} + 183.006\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (207). Entropy and heat capacity at 298 K estimated. High-temperature data based on Dworkin (69).

$HoCl_3(g)$

Holmium Trichloride (ideal gas)

[Formation: $Ho(c,l) + 1.5Cl_2(g) = HoCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.683	90.166	90.166	0	-163.100	-160.805	117.871
300	18.696	90.281	90.166	.035	-163.100	-160.790	117.134
400	19.177	95.734	90.907	1.931	-163.107	-160.021	87.430
500	19.417	100.042	92.318	3.862	-163.125	-159.244	69.605
600	19.553	103.595	93.910	5.811	-163.156	-158.467	57.721
700	19.640	106.616	95.515	7.771	-163.188	-157.683	49.230
800	19.704	109.243	97.070	9.738	-163.236	-156.893	42.861
900	19.759	111.567	98.554	11.712	-163.309	-156.092	37.904
1000	19.812	113.652	99.962	13.690	-163.415	-155.290	33.938
1100	19.869	115.543	101.294	15.674	-163.559	-154.477	30.691
1200	19.928	117.274	102.554	17.664	-163.751	-153.635	27.980
1300	19.991	118.871	103.748	19.660	-163.997	-152.783	25.685
1400	20.056	120.355	104.882	21.662	-164.306	-151.906	23.713
1500	20.121	121.741	105.960	23.671	-164.684	-151.006	22.001
1600	20.185	123.042	106.988	25.686	-165.141	-150.091	20.501
1700	20.247	124.267	107.968	27.708	-165.682	-149.124	19.171
1701	20.248	124.279	107.978	27.728	-165.688	-149.127	19.160
1701	20.248	124.279	107.978	27.728	-166.809	-149.127	19.160
1743	20.272	124.773	108.377	28.579	-166.813	-148.678	18.642
1743	20.272	124.773	108.377	28.579	-169.724	-148.678	18.642
1800	20.305	125.426	108.906	29.736	-169.945	-147.984	17.967
1900	20.360	126.526	109.805	31.769	-170.330	-146.767	16.882
2000	20.409	127.571	110.668	33.807	-170.715	-145.515	15.901

Phase changes: 1701 K, α - β transition point of Ho; $\Delta H°$ = 1.121 kcal/mol.
1743 K, melting point of Ho; $\Delta H°$ = 2.911 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.523 + 0.416\times10^{-3}T - 0.857\times10^{5}T^{-2}$

$H°- H°_{298} = 19.523\times10^{-3}T + 0.208\times10^{-6}T^2 + 0.857\times10^{2}T^{-1} - 6.127$

Formation equations (kcal/mol):

298.15-1701 K: $\Delta Hf° = -164.246 + 2.942\times10^{-3}T - 2.249\times10^{-6}T^2 + 139.950T^{-1}$

$\Delta Gf° = -164.246 - 2.942\times10^{-3}T\ln T + 2.249\times10^{-6}T^2 + 69.975T^{-1} + 26.846\times10^{-3}T$

1701-1743 K: $\Delta Hf° = -166.289 - 0.417\times10^{-3}T + 0.076\times10^{-6}T^2 - 16.750T^{-1}$

$\Delta Gf° = -166.289 + 0.417\times10^{-3}T\ln T - 0.076\times10^{-6}T^2 - 8.375T^{-1} + 7.041\times10^{-3}T$

1743-2000 K: $\Delta Hf° = -162.576 - 4.217\times10^{-3}T + 0.076\times10^{-6}T^2 - 16.750T^{-1}$

$\Delta Gf° = -162.576 + 4.217\times10^{-3}T\ln T - 0.076\times10^{-6}T^2 - 8.375T^{-1} - 23.449\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

HoF_3(c,l)

Holmium Trifluoride

[Formation: $Ho(c,l) + 1.5F_2(g) = HoF_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	21.800	28.400	28.400	0	-405.800	-387.257	283.863
300	21.821	28.535	28.402	.040	-405.793	-387.142	282.029
400	22.833	34.959	29.269	2.276	-405.368	-380.988	208.160
500	23.602	40.141	30.943	4.599	-404.921	-374.942	163.885
600	24.176	44.497	32.847	6.990	-404.452	-368.991	134.403
700	24.586	48.257	34.787	9.429	-403.960	-363.121	113.370
800	24.866	51.559	36.680	11.903	-403.466	-357.318	97.614
900	25.046	54.499	38.500	14.399	-402.987	-351.575	85.373
1000	25.159	57.144	40.235	16.909	-402.540	-345.891	75.594
1100	25.235	59.546	41.883	19.429	-402.132	-340.253	67.601
1200	25.306	61.744	43.447	21.956	-401.773	-334.635	60.945
1300	25.404	63.774	44.935	24.491	-401.470	-329.055	55.318
1343	25.462	64.601	45.550	25.585	-401.357	-326.660	53.158
1343	30.160	64.601	45.550	25.585	-401.357	-326.660	53.158
1400	30.160	65.855	46.352	27.304	-400.962	-323.497	50.500
1416	30.160	66.197	46.574	27.787	-400.855	-322.611	49.792
1416	22.940	75.703	46.574	41.247	-387.395	-322.611	49.792
1500	22.940	77.026	48.243	43.174	-387.474	-318.766	46.444
1600	22.940	78.506	50.088	45.468	-387.650	-314.189	42.916
1700	22.940	79.897	51.802	47.762	-387.917	-309.583	39.799
1701	22.940	79.910	51.818	47.785	-387.920	-309.549	39.771
1701	22.940	79.910	51.818	47.785	-389.041	-309.549	39.771
1743	22.940	80.470	52.502	48.748	-388.932	-307.575	38.565
1743	22.940	80.470	52.502	48.748	-391.843	-307.575	38.565
1800	22.940	81.208	53.399	50.056	-391.915	-304.815	37.009
1900	22.940	82.448	54.895	52.350	-392.041	-299.986	34.506
2000	22.940	83.625	56.303	54.644	-392.172	-295.136	32.251

*Entropy and heat capacity at 298 K estimated.

Phase changes: 1343 K, transition point of HoF_3; Some evidence indicates that transition is orthorhombic-hexagonal. Data insufficient to resolve enthalpy of transition of less than 0.200 kcal/mol.

1416 K, melting point of HoF_3; ΔH° = 13.460 kcal/mol.

1701 K, α - β transition point of Ho; ΔH° = 1.121 kcal/mol.

1743 K, melting point of Ho; ΔH° = 2.911 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1343 K: $Cp^\circ = 23.842 + 1.456\times10^{-3}T - 2.203\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 23.842\times10^{-3}T + 0.728\times10^{-6}T^2 + 2.203\times10^{2}T^{-1} - 7.912$

1343-1416 K: $Cp^\circ = 30.160$

$H^\circ - H^\circ_{298} = 30.160\times10^{-3}T - 14.920$

1416-2000 K: $Cp^\circ = 22.940$

$H^\circ - H^\circ_{298} = 22.940\times10^{-3}T + 8.764$

HoF_3(c,l) - Continued

Formation equations (kcal/mol):

298.15-1343 K: $\Delta Hf^\circ = -408.701 + 7.739\times10^{-3}T - 1.858\times10^{-6}T^2 + 226.250T^{-1}$

$\Delta Gf^\circ = -408.701 - 7.739\times10^{-3}T\ln T + 1.858\times10^{-6}T^2 + 113.125T^{-1} + 114.192\times10^{-3}T$

1343-1416 K: $\Delta Hf^\circ = -415.709 + 14.057\times10^{-3}T - 2.586\times10^{-6}T^2 + 5.950T^{-1}$

$\Delta Gf^\circ = -415.709 - 14.057\times10^{-3}T\ln T + 2.586\times10^{-6}T^2 + 2.975T^{-1} + 164.000\times10^{-3}T$

1416-1701 K: $\Delta Hf^\circ = -392.025 + 6.837\times10^{-3}T - 2.586\times10^{-6}T^2 + 5.950T^{-1}$

$\Delta Gf^\circ = -392.025 - 6.837\times10^{-3}T\ln T + 2.586\times10^{-6}T^2 + 2.975T^{-1} + 94.889\times10^{-3}T$

1701-1743 K: $\Delta Hf^\circ = -394.068 + 3.478\times10^{-3}T - 0.261\times10^{-6}T^2 - 150.750T^{-1}$

$\Delta Gf^\circ = -394.068 - 3.478\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 - 75.375T^{-1} + 75.084\times10^{-3}T$

1743-2000 K: $\Delta Hf^\circ = -390.355 - 0.322\times10^{-3}T - 0.261\times10^{-6}T^2 - 150.750T^{-1}$

$\Delta Gf^\circ = -390.355 + 0.322\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 - 75.375T^{-1} + 44.593\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Johnson (111). Entropy and heat capacity at 298 K estimated. High-temperature data based on Spedding (223).

$HoF_3(g)$

Holmium Trifluoride (ideal gas)

[Formation: $Ho(c,l) + 1.5F_2(g) = HoF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	17.016	81.776	81.776	0	-297.000	-294.371	215.777
300	17.041	81.882	81.776	.032	-297.001	-294.355	214.434
400	18.051	86.936	82.458	1.791	-297.054	-293.464	160.339
500	18.627	91.032	83.778	3.627	-297.093	-292.560	127.876
600	18.975	94.461	85.279	5.509	-297.133	-291.651	106.232
700	19.202	97.404	86.807	7.418	-297.171	-290.735	90.770
800	19.361	99.979	88.295	9.347	-297.222	-289.810	79.171
900	19.484	102.267	89.723	11.290	-297.296	-288.875	70.148
1000	19.588	104.325	91.082	13.243	-297.406	-287.938	62.928
1100	19.682	106.197	92.372	15.207	-297.554	-286.991	57.019
1200	19.770	107.913	93.597	17.179	-297.751	-286.015	52.090
1300	19.856	109.499	94.760	19.161	-298.000	-285.027	47.917
1400	19.939	110.974	95.866	21.151	-298.315	-284.017	44.336
1500	20.019	112.352	96.920	23.148	-298.701	-282.981	41.230
1600	20.095	113.646	97.925	25.154	-299.164	-281.927	38.509
1700	20.167	114.867	98.886	27.167	-299.712	-280.827	36.102
1701	20.168	114.879	98.896	27.187	-299.718	-280.828	36.081
1701	20.168	114.879	98.896	27.187	-300.839	-280.828	36.081
1743	20.196	115.371	99.287	28.035	-300.846	-280.321	35.148
1743	20.196	115.371	99.287	28.035	-303.757	-280.321	35.148
1800	20.234	116.022	99.807	29.187	-303.984	-279.550	33.942
1900	20.295	117.117	100.689	31.214	-304.377	-278.193	31.999
2000	20.351	118.160	101.537	33.246	-304.771	-276.805	30.247

Phase changes: 1701 K, α - β transition point of Ho; $\Delta H° = 1.121$ kcal/mol.
1743 K, melting point of Ho; $\Delta H° = 2.911$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.118 + 0.664\times10^{-3}T - 2.044\times10^{5}T^{-2}$

$H°-H°_{298} = 19.118\times10^{-3}T + 0.332\times10^{-6}T^2 + 2.044\times10^{2}T^{-1} - 6.415$

Formation equations (kcal/mol):

298.15-1701 K: $\Delta Hf° = -298.404 + 3.015\times10^{-3}T - 2.254\times10^{-6}T^2 + 210.350T^{-1}$

$\Delta Gf° = -298.404 - 3.015\times10^{-3}T\ln T + 2.254\times10^{-6}T^2 + 105.175T^{-1} + 28.851\times10^{-3}T$

1701-1743 K: $\Delta Hf° = -300.446 - 0.344\times10^{-3}T + 0.071\times10^{-6}T^2 + 53.650T^{-1}$

$\Delta Gf° = -300.446 + 0.344\times10^{-3}T\ln T - 0.071\times10^{-6}T^2 + 26.825T^{-1} + 9.046\times10^{-3}T$

1743-2000 K: $\Delta Hf° = -296.734 - 4.144\times10^{-3}T + 0.071\times10^{-6}T^2 + 53.650T^{-1}$

$\Delta Gf° = -296.734 + 4.144\times10^{-3}T\ln T - 0.071\times10^{-6}T^2 + 26.825T^{-1} - 21.445\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

$HoI_3(g)$

Holmium Triiodide (ideal gas)

[Formation: $Ho(c,l) + 1.5I_2(c,l,g) = HoI_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.468	103.341	103.341	0	-82.900	-95.951	70.333
300	19.473	103.461	103.341	.036	-82.912	-96.032	69.958
386.8	19.621	108.431	103.949	1.734	-83.597	-99.744	56.357
386.8	19.621	108.431	103.949	1.734	-89.160	-99.744	56.357
400	19.644	109.090	104.107	1.993	-89.371	-100.102	54.692
458.4	19.691	111.771	104.916	3.142	-90.300	-101.598	48.438
458.4	19.691	111.771	104.916	3.142	-105.331	-101.598	48.438
500	19.725	113.483	105.559	3.962	-105.349	-101.256	44.258
600	19.771	117.084	107.189	5.937	-105.396	-100.436	36.583
700	19.801	120.134	108.825	7.916	-105.440	-99.605	31.098
800	19.828	122.780	110.409	9.897	-105.497	-98.765	26.981
900	19.858	125.117	111.916	11.881	-105.581	-97.917	23.777
1000	19.893	127.211	113.342	13.869	-105.693	-97.062	21.213
1100	19.935	129.109	114.691	15.860	-105.846	-96.199	19.113
1200	19.984	130.845	115.965	17.856	-106.045	-95.305	17.357
1300	20.039	132.447	117.172	19.857	-106.297	-94.402	15.870
1400	20.097	133.934	118.317	21.864	-106.613	-93.471	14.591
1500	20.157	135.323	119.405	23.877	-106.997	-92.520	13.480
1600	20.217	136.626	120.442	25.895	-107.460	-91.548	12.505
1700	20.275	137.853	121.429	27.920	-108.008	-90.531	11.638
1701	20.276	137.865	121.439	27.940	-108.014	-90.533	11.632
1701	20.276	137.865	121.439	27.940	-109.135	-90.533	11.632
1743	20.299	138.360	121.841	28.792	-109.142	-90.061	11.292
1743	20.299	138.360	121.841	28.792	-112.053	-90.061	11.292
1800	20.330	139.013	122.374	29.950	-112.279	-89.335	10.847
1900	20.382	140.114	123.279	31.986	-112.671	-88.064	10.130
2000	20.429	141.161	124.148	34.026	-113.061	-86.757	9.480

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
1701 K, α - β transition point of Ho; $\Delta H°$ = 1.121 kcal/mol.
1743 K, melting point of Ho; $\Delta H°$ = 2.911 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.572 + 0.392\times10^{-3}T - 0.196\times10^{5}T^{-2}$

$H°- H°_{298} = 19.572\times10^{-3}T + 0.196\times10^{-6}T^{2} + 0.196\times10^{2}T^{-1} - 5.919$

$HoI_3(g)$ - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -82.183 - 3.084\times10^{-3}T - 4.367\times10^{-6}T^2 + 176.300T^{-1}$

$\Delta Gf^\circ = -82.183 + 3.084\times10^{-3}T\ln T + 4.367\times10^{-6}T^2 + 88.150T^{-1} - 66.045\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -84.366 - 12.690\times10^{-3}T - 2.129\times10^{-6}T^2 + 176.300T^{-1}$

$\Delta Gf^\circ = -84.366 + 12.690\times10^{-3}T\ln T + 2.129\times10^{-6}T^2 + 88.150T^{-1} - 116.768\times10^{-3}T$

458.4-1701 K: $\Delta Hf^\circ = -106.436 + 2.820\times10^{-3}T - 2.231\times10^{-6}T^2 + 153.350T^{-1}$

$\Delta Gf^\circ = -106.436 - 2.820\times10^{-3}T\ln T + 2.231\times10^{-6}T^2 + 76.675T^{-1} + 26.426\times10^{-3}T$

1701-1743 K: $\Delta Hf^\circ = -108.478 - 0.539\times10^{-3}T + 0.094\times10^{-6}T^2 - 3.350T^{-1}$

$\Delta Gf^\circ = -108.478 + 0.539\times10^{-3}T\ln T - 0.094\times10^{-6}T^2 - 1.675T^{-1} + 6.621\times10^{-3}T$

1743-2000 K: $\Delta Hf^\circ = -104.766 - 4.339\times10^{-3}T + 0.094\times10^{-6}T^2 - 3.350T^{-1}$

$\Delta Gf^\circ = -104.766 + 4.339\times10^{-3}T\ln T - 0.094\times10^{-6}T^2 - 1.675T^{-1} - 23.869\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166)and Schumm (207). Other data based on Myers (165) and Dieke (56).

IBr(g)

Iodine Monobromide (ideal gas)

[Formation: $0.5I_2(c,l,g) + 0.5Br_2(l,g) = IBr(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.731	61.864	61.864	0	9.770	0.886	-0.650
300	8.734	61.918	61.865	.016	9.758	.832	-.606
332.6	8.773	62.821	61.915	.301	9.530	-.127	.083
332.6	8.773	62.821	61.915	.301	5.997	-.127	.083
386.8	8.837	64.152	62.138	.779	5.854	-1.116	.630
386.8	8.837	64.152	62.138	.779	3.999	-1.116	.630
400	8.853	64.449	62.209	.896	3.931	-1.289	.704
458.4	8.892	65.658	62.573	1.415	3.629	-2.029	.967
458.4	8.892	65.658	62.573	1.415	-1.381	-2.029	.967
500	8.919	66.432	62.862	1.785	-1.380	-2.087	.912
600	8.961	68.062	63.597	2.679	-1.379	-2.229	.812
700	8.993	69.446	64.336	3.577	-1.377	-2.371	.740
800	9.019	70.649	65.052	4.478	-1.374	-2.512	.686
900	9.041	71.712	65.733	5.381	-1.372	-2.655	.645
1000	9.061	72.666	66.380	6.286	-1.370	-2.797	.611
1100	9.080	73.530	66.991	7.193	-1.368	-2.940	.584
1200	9.098	74.321	67.569	8.102	-1.364	-3.083	.561
1300	9.116	75.050	68.118	9.012	-1.361	-3.227	.543
1400	9.136	75.726	68.637	9.925	-1.357	-3.369	.526
1500	9.159	76.357	69.130	10.840	-1.353	-3.514	.512
1600	9.186	76.949	69.601	11.757	-1.347	-3.657	.500
1700	9.220	77.507	70.050	12.677	-1.340	-3.803	.489
1800	9.261	78.035	70.479	13.601	-1.330	-3.948	.479
1900	9.312	78.537	70.890	14.530	-1.317	-4.092	.471
2000	9.374	79.017	71.285	15.464	-1.300	-4.241	.463

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.918 + 0.168\times10^{-3}T - 0.211\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.918\times10^{-3}T + 0.084\times10^{-6}T^2 + 0.211\times10^{2}T^{-1} - 2.737$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = 11.711 - 6.566\times10^{-3}T - 0.612\times10^{-6}T^2 + 21.100T^{-1}$

$\Delta Gf^\circ = 11.711 + 6.566\times10^{-3}T\ln T + 0.612\times10^{-6}T^2 + 10.550T^{-1} - 74.018\times10^{-3}T$

332.6-386.8 K: $\Delta Hf^\circ = 6.711 - 1.985\times10^{-3}T - 0.689\times10^{-6}T^2 + 5.400T^{-1}$

$\Delta Gf^\circ = 6.711 + 1.985\times10^{-3}T\ln T + 0.689\times10^{-6}T^2 + 2.700T^{-1} - 32.341\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = 5.984 - 5.188\times10^{-3}T + 0.056\times10^{-6}T^2 + 5.400T^{-1}$

$\Delta Gf^\circ = 5.984 + 5.188\times10^{-3}T\ln T - 0.056\times10^{-6}T^2 + 2.700T^{-1} - 49.248\times10^{-3}T$

458.4-2000 K: $\Delta Hf^\circ = -1.373 - 0.018\times10^{-3}T + 0.022\times10^{-6}T^2 - 2.250T^{-1}$

$\Delta Gf^\circ = -1.373 + 0.018\times10^{-3}T\ln T - 0.022\times10^{-6}T^2 - 1.125T^{-1} - 1.517\times10^{-3}T$

Source: Data from JANAF (60).

ICl(c,l)

Iodine Monochloride

[Formation: $0.5I_2(c) + 0.5Cl_2(g) = ICl(s,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	13.200	23.405	23.405	0	-8.510	-3.406	2.497
300	13.223	23.487	23.407	.024	-8.505	-3.375	2.458
300.53	13.229	23.509	23.406	.031	-8.504	-3.365	2.447
300.53	24.588	32.739	23.406	2.805	-5.730	-3.365	2.447
370	23.860	37.808	25.646	4.500	-4.797	-2.918	1.724

Phase changes: 300.53 melting point of ICl; ΔH° = 2.774 kcal/mol.
370 K, ICl vaporizes with decomposition.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-300.53 K: $Cp^\circ = 13.200$

$H^\circ - H^\circ_{298} = 13.200\times10^{-3}T - 3.936$

300.53-370 K: $Cp^\circ = 26.225 - 5.440\times10^{-3}T$

$H^\circ - H^\circ_{298} = 26.225\times10^{-3}T - 2.720\times10^{-6}T^2 - 4.831$

Formation equations (kcal/mol):

298.15-300.53 K: $\Delta Hf^\circ = -9.025 + 2.348\times10^{-3}T - 0.790\times10^{-6}T^2 - 34.150T^{-1}$

$\Delta Gf^\circ = -9.025 - 2.348\times10^{-3}T\ln T + 0.790\times10^{-6}T^2 - 17.075T^{-1} + 32.182\times10^{-3}T$

300.53-370 K: $\Delta Hf^\circ = -9.920 + 15.373\times10^{-3}T - 3.510\times10^{-6}T^2 - 34.150T^{-1}$

$\Delta Gf^\circ = -9.920 - 15.373\times10^{-3}T\ln T + 3.510\times10^{-6}T^2 - 17.075T^{-1} + 108.656\times10^{-3}T$

Sources: Data based on Calder (20) and Lamoreaux (139).

ICl(g)
Iodine Monochloride (ideal gas)
[Formation: $0.5I_2(c,l,g) + 0.5Cl_2(g) = ICl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.497	59.145	59.145	0	4.110	-1.442	1.057
300	8.502	59.198	59.145	.016	4.107	-1.476	1.075
386.8	8.674	61.382	59.412	.762	3.889	-3.065	1.732
386.8	8.674	61.382	59.412	.762	2.035	-3.065	1.732
400	8.700	61.674	59.481	.877	1.966	-3.238	1.769
458.4	8.763	62.865	59.838	1.388	1.667	-3.975	1.895
458.4	8.763	62.865	59.838	1.388	-3.344	-3.975	1.895
500	8.808	63.628	60.122	1.753	-3.343	-4.031	1.762
600	8.873	65.240	60.845	2.637	-3.342	-4.170	1.519
700	8.918	66.611	61.572	3.527	-3.340	-4.308	1.345
800	8.952	67.805	62.280	4.420	-3.341	-4.447	1.215
900	8.978	68.860	62.952	5.317	-3.341	-4.584	1.113
1000	9.000	69.808	63.592	6.216	-3.341	-4.723	1.032
1100	9.019	70.666	64.196	7.117	-3.343	-4.860	.966
1200	9.036	71.452	64.769	8.020	-3.344	-4.999	.910
1300	9.052	72.176	65.311	8.924	-3.345	-5.137	.864
1400	9.066	72.847	65.826	9.830	-3.347	-5.274	.823
1500	9.080	73.473	66.315	10.737	-3.350	-5.412	.789
1600	9.094	74.059	66.780	11.646	-3.352	-5.548	.758
1700	9.106	74.611	67.225	12.556	-3.354	-5.685	.731
1800	9.119	75.132	67.650	13.467	-3.358	-5.824	.707
1900	9.131	75.625	68.057	14.380	-3.360	-5.958	.685
2000	9.143	76.094	68.448	15.293	-3.365	-6.096	.666

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 8.904 + 0.130\times10^{-3}T - 0.396\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.904\times10^{-3}T + 0.065\times10^{-6}T^2 + 0.396\times10^{2}T^{-1} - 2.793$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = 4.737 - 1.948\times10^{-3}T - 0.725\times10^{-6}T^2 + 5.450T^{-1}$

$\Delta Gf^\circ = 4.737 + 1.948\times10^{-3}T\ln T + 0.725\times10^{-6}T^2 + 2.725T^{-1} - 32.070\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = 4.009 - 5.150\times10^{-3}T + 0.021\times10^{-6}T^2 + 5.450T^{-1}$

$\Delta Gf^\circ = 4.009 + 5.150\times10^{-3}T\ln T - 0.021\times10^{-6}T^2 + 2.725T^{-1} - 48.977\times10^{-3}T$

458.4-2000 K: $\Delta Hf^\circ = -3.347 + 0.020\times10^{-3}T - 0.013\times10^{-6}T^2 - 2.200T^{-1}$

$\Delta Gf^\circ = -3.347 - 0.020\times10^{-3}T\ln T + 0.013\times10^{-6}T^2 - 1.100T^{-1} - 1.246\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Calder (20) and Lamoreaux (139). Other data from JANAF (60).

IF(g)

Iodine Monofluoride (ideal gas)

[Formation: $0.5I_2(c,l,g) + 0.5F_2(g) = IF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.021	56.451	56.451	0	-22.648	-28.119	20.612
300	8.030	56.501	56.451	.015	-22.652	-28.153	20.509
386.8	8.337	58.583	56.705	.727	-22.877	-29.717	16.790
386.8	8.337	58.583	56.705	.727	-24.732	-29.717	16.790
400	8.384	58.864	56.771	.837	-24.801	-29.886	16.329
458.4	8.511	60.017	57.113	1.331	-25.102	-30.606	14.592
458.4	8.511	60.017	57.113	1.331	-30.113	-30.606	14.592
500	8.601	60.760	57.386	1.687	-30.112	-30.650	13.397
600	8.743	62.341	58.083	2.555	-30.107	-30.758	11.203
700	8.841	63.696	58.790	3.434	-30.102	-30.867	9.637
800	8.915	64.882	59.480	4.322	-30.095	-30.977	8.462
900	8.973	65.936	60.139	5.217	-30.088	-31.087	7.549
1000	9.020	66.883	60.767	6.116	-30.081	-31.199	6.818
1100	9.061	67.745	61.363	7.020	-30.074	-31.312	6.221
1200	9.097	68.535	61.928	7.928	-30.066	-31.425	5.723
1300	9.130	69.265	62.465	8.840	-30.056	-31.537	5.302
1400	9.160	69.942	62.975	9.754	-30.048	-31.652	4.941
1500	9.188	70.575	63.460	10.672	-30.038	-31.767	4.628
1600	9.215	71.169	63.924	11.592	-30.028	-31.882	4.355
1700	9.241	71.729	64.367	12.515	-30.017	-31.999	4.114
1800	9.266	72.258	64.791	13.440	-30.006	-32.117	3.899
1900	9.290	72.759	65.197	14.368	-29.994	-32.232	3.708
2000	9.313	73.236	65.587	15.298	-29.983	-32.350	3.535

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.749 + 0.320\times10^{-3}T - 0.732\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.749\times10^{-3}T + 0.160\times10^{-6}T^2 + 0.732\times10^{2}T^{-1} - 2.868$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -22.086 - 1.944\times10^{-3}T - 0.673\times10^{-6}T^2 + 22.950T^{-1}$

$\Delta Gf^\circ = -22.086 + 1.944\times10^{-3}T\ln T + 0.673\times10^{-6}T^2 + 11.475T^{-1} - 31.640\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -22.813 - 5.146\times10^{-3}T + 0.073\times10^{-6}T^2 + 22.950T^{-1}$

$\Delta Gf^\circ = -22.813 + 5.146\times10^{-3}T\ln T - 0.073\times10^{-6}T^2 + 11.475T^{-1} - 48.547\times10^{-3}T$

458.4-2000 K: $\Delta Hf^\circ = -30.170 + 0.024\times10^{-3}T + 0.039\times10^{-6}T^2 + 15.300T^{-1}$

$\Delta Gf^\circ = -30.170 - 0.024\times10^{-3}T\ln T - 0.039\times10^{-6}T^2 + 7.650T^{-1} - 0.816\times10^{-3}T$

Source: Data from JANAF (60).

$IF_5(g)$

Iodine Pentafluoride (ideal gas)

[Formation: $0.5I_2(c,l,g) + 2.5F_2(g) = IF_5(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	24.588	79.959	79.959	0	-200.840	-184.434	135.192
300	24.651	80.111	79.959	.046	-200.841	-184.332	134.284
386.8	26.853	86.679	80.750	2.293	-200.861	-179.550	101.448
386.8	26.853	86.679	80.750	2.293	-202.715	-179.550	101.448
400	27.188	87.586	80.961	2.650	-202.745	-178.760	97.668
458.4	28.033	91.361	82.049	4.268	-202.855	-175.248	83.551
458.4	28.033	91.361	82.049	4.268	-207.866	-175.248	83.551
500	28.635	93.822	82.928	5.447	-207.717	-172.294	75.309
600	29.512	99.127	85.197	8.358	-207.330	-165.247	60.190
700	30.076	103.721	87.522	11.339	-206.918	-158.265	49.412
800	30.457	107.764	89.805	14.367	-206.496	-151.344	41.345
900	30.726	111.367	92.004	17.427	-206.065	-144.473	35.082
1000	30.922	114.615	94.105	20.510	-205.635	-137.655	30.084
1100	31.069	117.570	96.106	23.610	-205.203	-130.877	26.003
1200	31.182	120.278	98.009	26.723	-204.773	-124.139	22.609
1300	31.271	122.778	99.820	29.845	-204.342	-117.436	19.743
1400	31.342	125.098	101.544	32.976	-203.917	-110.770	17.292
1500	31.399	127.262	103.187	36.113	-203.495	-104.131	15.172
1600	31.446	129.290	104.755	39.256	-203.074	-97.518	13.320
1700	31.486	131.198	106.256	42.402	-202.656	-90.933	11.690
1800	31.519	132.999	107.692	45.553	-202.243	-84.374	10.244
1900	31.547	134.703	109.068	48.706	-201.832	-77.834	8.953
2000	31.571	136.322	110.391	51.862	-201.428	-71.320	7.793

Phase changes: 282.57 K, melting point of IF_5; $\Delta H°$ = 2.680 kcal/mol.
377.63 K, boiling point of IF_5; $\Delta H°$ = 8.60 kcal/mol.
386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 30.566 + 0.740\times10^{-3}T - 5.510\times10^{5}T^{-2}$

$H°- H°_{298} = 30.566\times10^{-3}T + 0.370\times10^{-6}T^2 + 5.510\times10^{2}T^{-1} - 10.994$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -202.625 + 2.857\times10^{-3}T - 0.811\times10^{-6}T^2 + 299.750T^{-1}$

$\Delta Gf° = -202.625 - 2.857\times10^{-3}T\ln T + 0.811\times10^{-6}T^2 + 149.875T^{-1} + 75.368\times10^{-3}T$

386.8-458.4 K: $\Delta Hf° = -203.353 - 0.345\times10^{-3}T + 0.065\times10^{-6}T^2 + 299.750T^{-1}$

$\Delta Gf° = -203.353 + 0.345\times10^{-3}T\ln T + 0.065\times10^{-6}T^2 + 149.875T^{-1} + 58.461\times10^{-3}T$

458.4-2000 K: $\Delta Hf° = -210.709 + 4.825\times10^{-3}T - 0.099\times10^{-6}T^2 + 292.100T^{-1}$

$\Delta Gf° = -210.709 - 4.825\times10^{-3}T\ln T + 0.099\times10^{-6}T^2 + 146.050T^{-1} + 106.192\times10^{-3}T$

Sources: Data from JANAF (60) who estimated some molecular constants. Fusion and boiling data from Osborne (180).

$IF_7(g)$

Iodine Heptafluoride (ideal gas)

[Formation: $0.5I_2(c,l,g) + 3.5F_2(g) = IF_7(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	32.134	83.085	83.085	0	-229.700	-199.782	146.442
300	32.235	83.284	83.085	.060	-229.701	-199.597	145.404
386.8	35.783	91.965	84.126	3.032	-229.661	-190.887	107.854
386.8	35.783	91.965	84.126	3.032	-231.516	-190.887	107.854
400	36.323	93.175	84.405	3.508	-231.531	-189.500	103.537
458.4	37.679	98.238	85.850	5.678	-231.554	-183.360	87.419
458.4	37.679	98.238	85.850	5.678	-236.565	-183.360	87.419
500	38.645	101.553	87.021	7.266	-236.345	-178.541	78.039
600	40.052	108.733	90.055	11.207	-235.758	-167.035	60.842
700	40.957	114.980	93.180	15.260	-235.122	-155.632	48.590
800	41.569	120.491	96.256	19.388	-234.462	-144.322	39.427
900	42.001	125.414	99.227	23.568	-233.783	-133.092	32.319
1000	42.315	129.856	102.071	27.785	-233.098	-121.944	26.650
1100	42.552	133.901	104.784	32.029	-232.409	-110.860	22.026
1200	42.733	137.611	107.367	36.293	-231.717	-99.842	18.183
1300	42.876	141.037	109.826	40.574	-231.023	-88.876	14.941
1400	42.990	144.219	112.171	44.867	-230.337	-77.973	12.172
1500	43.082	147.188	114.407	49.171	-229.649	-67.114	9.778
1600	43.158	149.971	116.544	53.483	-228.965	-56.298	7.690
1700	43.221	152.590	118.589	57.802	-228.283	-45.526	5.853
1800	43.274	155.062	120.547	62.127	-227.608	-34.796	4.225
1900	43.319	157.403	122.426	66.457	-226.933	-24.100	2.772
2000	43.358	159.626	124.231	70.791	-226.269	-13.444	1.469

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 41.758 + 1.178\times10^{-3}T - 8.867\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 41.758\times10^{-3}T + 0.589\times10^{-6}T^2 + 8.867\times10^{2}T^{-1} - 15.477$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -233.078 + 5.541\times10^{-3}T - 0.766\times10^{-6}T^2 + 534.950T^{-1}$

$\Delta Gf^\circ = -233.078 - 5.541\times10^{-3}T\ln T + 0.766\times10^{-6}T^2 + 267.475T^{-1} + 140.011\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -233.806 + 2.339\times10^{-3}T - 0.020\times10^{-6}T^2 + 534.950T^{-1}$

$\Delta Gf^\circ = -233.806 - 2.339\times10^{-3}T\ln T + 0.020\times10^{-6}T^2 + 267.475T^{-1} + 123.104\times10^{-3}T$

458.4-2000 K: $\Delta Hf^\circ = -241.163 + 7.510\times10^{-3}T - 0.054\times10^{-6}T^2 + 527.300T^{-1}$

$\Delta Gf^\circ = -241.163 - 7.510\times10^{-3}T\ln T + 0.054\times10^{-6}T^2 + 263.650T^{-1} + 170.835\times10^{-3}T$

Source: Data from JANAF (60).

InCl(c,l)
Indium Monochloride
[Formation: $In(c,l) + 0.5Cl_2(g) = InCl(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.299	23.901	23.901	0	-44.460	-39.521	28.970
300	12.312	23.977	23.901	.023	-44.457	-39.491	28.769
387	12.906	27.183	24.289	1.120	-44.294	-38.073	21.501
387	13.384	27.506	24.289	1.245	-44.169	-38.073	21.501
400	13.384	27.948	24.400	1.419	-44.139	-37.868	20.690
429.78	13.384	28.909	24.680	1.818	-44.077	-37.404	19.020
429.78	13.384	28.909	24.680	1.818	-44.857	-37.404	19.020
484	13.384	30.499	25.245	2.543	-44.745	-36.470	16.468
484	16.013	41.016	25.245	7.633	-39.655	-36.470	16.468
500	16.013	41.538	25.760	7.889	-39.580	-36.367	15.896
600	16.013	44.458	28.640	9.491	-39.114	-35.767	13.028
700	16.013	46.926	31.080	11.092	-38.653	-35.246	11.004
800	16.013	49.064	33.198	12.693	-38.193	-34.792	9.505
900	16.013	50.951	35.068	14.295	-37.731	-34.394	8.352
1000	16.013	52.638	36.742	15.896	-37.272	-34.049	7.441
1100	16.013	54.164	38.258	17.497	-36.815	-33.748	6.705
1200	16.013	55.557	39.641	19.099	-36.358	-33.489	6.099

Phase changes: 387 K, α - β transition point of InCl; ΔH° = 0.125 kcal/mol.
429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.
484 K, melting point of InCl; ΔH° = 5.090 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-387 K: $Cp^\circ = 10.241 + 6.900\times10^{-3}T$
$H^\circ - H^\circ_{298} = 10.241\times10^{-3}T + 3.450\times10^{-6}T^2 - 3.360$

387-484 K: $Cp^\circ = 13.384$
$H^\circ - H^\circ_{298} = 13.384\times10^{-3}T - 3.935$

484-1200 K: $Cp^\circ = 16.013$
$H^\circ - H^\circ_{298} = 16.013\times10^{-3}T - 0.117$

Formation equations (kcal/mol):

298.15-387 K: $\Delta Hf^\circ = -45.459 + 3.207\times10^{-3}T - 1.356\times10^{-6}T^2 + 48.550T^{-1}$
$\Delta Gf^\circ = -45.459 - 3.207\times10^{-3}T\ln T + 1.356\times10^{-6}T^2 + 24.275T^{-1} + 37.511\times10^{-3}T$

387-429.78 K: $\Delta Hf^\circ = -46.033 + 6.350\times10^{-3}T - 4.806\times10^{-6}T^2 + 48.550T^{-1}$
$\Delta Gf^\circ = -46.033 - 6.350\times10^{-3}T\ln T + 4.806\times10^{-6}T^2 + 24.275T^{-1} + 56.388\times10^{-3}T$

429.78-484 K: $\Delta Hf^\circ = -45.674 + 2.003\times10^{-3}T - 0.034\times10^{-6}T^2 - 17.150T^{-1}$
$\Delta Gf^\circ = -45.674 - 2.003\times10^{-3}T\ln T + 0.034\times10^{-6}T^2 - 8.575T^{-1} + 31.423\times10^{-3}T$

484-1200 K: $\Delta Hf^\circ = -41.856 + 4.633\times10^{-3}T - 0.034\times10^{-6}T^2 - 17.150T^{-1}$
$\Delta Gf^\circ = -41.856 - 4.633\times10^{-3}T\ln T + 0.034\times10^{-6}T^2 - 8.575T^{-1} + 39.788\times10^{-3}T$

Source: Data from Gurvich (95).

InCl(g)

Indium Monochloride (ideal gas)

[Formation: $In(c,l) + 0.5Cl_2(g) = InCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.637	59.312	59.312	0	-17.120	-22.739	16.668
300	8.641	59.365	59.312	.016	-17.124	-22.774	16.591
400	8.793	61.875	59.653	.889	-17.330	-24.629	13.457
429.78	8.817	62.507	59.829	1.151	-17.403	-25.170	12.799
429.78	8.817	62.507	59.829	1.151	-18.183	-25.170	12.799
500	8.875	63.847	60.303	1.772	-18.357	-26.298	11.495
600	8.928	65.470	61.032	2.663	-18.603	-27.863	10.149
700	8.966	66.849	61.766	3.558	-18.847	-29.386	9.175
800	8.996	68.048	62.478	4.456	-19.090	-30.876	8.435
900	9.021	69.109	63.157	5.357	-19.330	-32.334	7.852
1000	9.044	70.061	63.801	6.260	-19.569	-33.767	7.380
1100	9.065	70.924	64.410	7.165	-19.807	-35.176	6.989
1200	9.085	71.714	64.986	8.073	-20.044	-36.563	6.659
1300	9.105	72.442	65.533	8.982	-20.281	-37.931	6.377
1400	9.124	73.117	66.050	9.894	-20.516	-39.277	6.131
1500	9.143	73.747	66.542	10.807	-20.751	-40.609	5.917
1600	9.162	74.338	67.011	11.723	-20.984	-41.926	5.727
1700	9.181	74.894	67.459	12.640	-21.217	-43.226	5.557
1800	9.201	75.419	67.886	13.559	-21.448	-44.516	5.405
1900	9.221	75.917	68.296	14.480	-21.678	-45.790	5.267
2000	9.241	76.391	68.689	15.403	-21.908	-47.055	5.142

Phase change: 429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.907 + 0.166\times10^{-3}T - 0.284\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.907\times10^{-3}T + 0.083\times10^{-6}T^2 + 0.284\times10^{2}T^{-1} - 2.758$

Formation equations (kcal/mol):

298.15-429.78 K: $\Delta Hf^\circ = -17.517 + 1.873\times10^{-3}T - 4.723\times10^{-6}T^2 + 76.950T^{-1}$

$\Delta Gf^\circ = -17.517 - 1.873\times10^{-3}T\ln T + 4.723\times10^{-6}T^2 + 38.475T^{-1} - 8.683\times10^{-3}T$

429.78-2000 K: $\Delta Hf^\circ = -17.157 - 2.474\times10^{-3}T + 0.049\times10^{-6}T^2 + 11.250T^{-1}$

$\Delta Gf^\circ = -17.157 + 2.474\times10^{-3}T\ln T - 0.049\times10^{-6}T^2 + 5.625T^{-1} - 33.648\times10^{-3}T$

Source: Data from Gurvich (95).

$InCl_2(g)$
Indium Dichloride (ideal gas)
[Formation: $In(c,l) + Cl_2(g) = InCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.937	74.544	74.544	0	-53.080	-55.296	40.533
300	12.947	74.624	74.544	.024	-53.083	-55.310	40.293
400	13.332	78.408	75.058	1.340	-53.261	-56.029	30.612
429.78	13.390	79.367	75.324	1.738	-53.325	-56.232	28.595
429.78	13.390	79.367	75.324	1.738	-54.105	-56.232	28.595
500	13.528	81.406	76.038	2.684	-54.254	-56.568	24.725
600	13.640	83.883	77.145	4.043	-54.466	-57.010	20.766
700	13.710	85.992	78.262	5.411	-54.676	-57.418	17.926
800	13.756	87.826	79.346	6.784	-54.887	-57.797	15.789
900	13.788	89.448	80.380	8.161	-55.096	-58.147	14.120
1000	13.811	90.902	81.361	9.541	-55.305	-58.476	12.780
1100	13.828	92.219	82.288	10.924	-55.514	-58.781	11.679
1200	13.843	93.423	83.167	12.307	-55.726	-59.070	10.758
1300	13.855	94.531	83.999	13.692	-55.938	-59.340	9.976
1400	13.866	95.558	84.788	15.078	-56.151	-59.592	9.303
1500	13.878	96.515	85.538	16.465	-56.365	-59.830	8.717
1600	13.891	97.412	86.253	17.854	-56.579	-60.056	8.203
1700	13.906	98.254	86.935	19.243	-56.794	-60.264	7.747
1800	13.922	99.049	87.585	20.635	-57.008	-60.464	7.341
1900	13.941	99.803	88.209	22.028	-57.222	-60.650	6.976
2000	13.962	100.518	88.806	23.423	-57.437	-60.825	6.647

Phase change: 429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.817 + 0.068\times10^{-3}T - 0.801\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.817\times10^{-3}T + 0.034\times10^{-6}T^2 + 0.801\times10^{2}T^{-1} - 4.391$

Formation equations (kcal/mol):

298.15-429.78 K: $\Delta Hf^\circ = -53.675 + 2.370\times10^{-3}T - 4.816\times10^{-6}T^2 + 94.500T^{-1}$

$\Delta Gf^\circ = -53.675 - 2.370\times10^{-3}T\ln T + 4.816\times10^{-6}T^2 + 47.250T^{-1} + 6.099\times10^{-3}T$

429.78-2000 K: $\Delta Hf^\circ = -53.316 - 1.977\times10^{-3}T - 0.044\times10^{-6}T^2 + 28.800T^{-1}$

$\Delta Gf^\circ = -53.316 + 1.977\times10^{-3}T\ln T + 0.044\times10^{-6}T^2 + 14.400T^{-1} - 18.866\times10^{-3}T$

Source: Data from Gurvich (95).

$InCl_3(g)$

Indium Trichloride (ideal gas)

[Formation: $In(c,l) + 1.5Cl_2(g) = InCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	18.330	81.560	81.560	0	-89.400	-85.764	62.866
300	18.350	81.670	81.570	.030	-89.405	-85.745	62.464
400	18.960	87.050	82.300	1.900	-89.443	-84.523	46.181
429.78	19.049	88.415	82.677	2.466	-89.466	-84.156	42.794
429.78	19.049	88.415	82.677	2.466	-90.246	-84.156	42.794
500	19.260	91.310	83.690	3.810	-90.297	-83.155	36.347
600	19.440	94.840	85.257	5.750	-90.363	-81.717	29.765
700	19.550	97.850	86.850	7.700	-90.430	-80.274	25.062
800	19.620	100.470	88.395	9.660	-90.497	-78.822	21.533
900	19.670	102.780	89.869	11.620	-90.567	-77.359	18.785
1000	19.710	104.860	91.270	13.590	-90.634	-75.894	16.586
1100	19.730	106.740	92.595	15.560	-90.704	-74.418	14.785
1200	19.750	108.450	93.842	17.530	-90.779	-72.930	13.282
1300	19.770	110.040	95.032	19.510	-90.847	-71.447	12.011
1400	19.780	111.500	96.150	21.490	-90.918	-69.940	10.918
1500	19.790	112.870	97.223	23.470	-90.992	-68.445	9.972
1600	19.800	114.150	98.244	25.450	-91.069	-66.943	9.144
1700	19.810	115.350	99.215	27.430	-91.148	-65.429	8.411
1800	19.810	116.480	100.141	29.410	-91.229	-63.915	7.760
1900	19.820	117.550	101.029	31.390	-91.312	-62.391	7.177
2000	19.820	118.570	101.885	33.370	-91.400	-60.877	6.652

Phase change: 429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.749 + 0.066\times10^{-3}T - 1.279\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.749\times10^{-3}T + 0.033\times10^{-6}T^2 + 1.279\times10^{2}T^{-1} - 6.320$

Formation equations (kcal/mol):

298.15-429.78 K: $\Delta Hf^\circ = -90.490 + 3.889\times10^{-3}T - 4.861\times10^{-6}T^2 + 108.150T^{-1}$

$\Delta Gf^\circ = -90.490 - 3.889\times10^{-3}T\ln T + 4.861\times10^{-6}T^2 + 54.075T^{-1} + 35.948\times10^{-3}T$

429.78-2000 K: $\Delta Hf^\circ = -90.130 - 0.458\times10^{-3}T - 0.089\times10^{-6}T^2 + 42.450T^{-1}$

$\Delta Gf^\circ = -90.130 + 0.458\times10^{-3}T\ln T + 0.089\times10^{-6}T^2 + 21.225T^{-1} + 10.983\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Other data from Givan (89).

$(InCl_3)_2(g)$
Dimeric Indium Trichloride (ideal gas)
[Formation: $2In(c,l) + 3Cl_2(g) = (InCl_3)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	40.384	126.406	126.406	0	-211.440	-193.222	141.634
300	40.420	126.656	126.406	.075	-211.434	-193.109	140.678
400	41.765	138.493	128.010	4.193	-211.134	-187.051	102.198
429.78	41.965	141.499	128.842	5.440	-211.064	-185.260	94.206
429.78	41.965	141.499	128.842	5.440	-212.624	-185.260	94.206
500	42.437	147.892	131.080	8.406	-212.448	-180.800	79.027
600	42.816	155.666	134.549	12.670	-212.195	-174.495	63.559
700	43.050	162.285	138.049	16.965	-211.934	-168.232	52.524
800	43.204	168.045	141.447	21.278	-211.675	-162.010	44.259
900	43.311	173.140	144.691	25.604	-211.411	-155.815	37.837
1000	43.387	177.707	147.768	29.939	-211.148	-149.655	32.707
1100	43.444	181.845	150.680	34.281	-210.887	-143.516	28.514
1200	43.488	185.627	153.438	38.627	-210.631	-137.406	25.025
1300	43.521	189.110	156.050	42.978	-210.376	-131.315	22.076
1400	43.548	192.336	158.528	47.331	-210.125	-125.240	19.551
1500	43.570	195.341	160.883	51.687	-209.877	-119.184	17.365
1600	43.588	198.154	163.126	56.045	-209.633	-113.148	15.455
1700	43.603	200.798	165.266	60.405	-209.390	-107.120	13.771
1800	43.615	203.290	167.309	64.766	-209.152	-101.118	12.277
1900	43.626	205.648	169.265	69.128	-208.916	-95.116	10.941
2000	43.635	207.886	171.141	73.491	-208.688	-89.136	9.740

Phase change: 429.78 K, melting point of In; $\Delta H° = 0.780$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 43.538 + 0.106\times10^{-3}T - 2.832\times10^{5}T^{-2}$

$H°- H°_{298} = 43.538\times10^{-3}T + 0.053\times10^{-6}T^2 + 2.832\times10^{2}T^{-1} - 13.935$

Formation equations (kcal/mol):

298.15-429.78 K: $\Delta Hf° = -214.915 + 11.817\times10^{-3}T - 9.735\times10^{-6}T^2 + 243.700T^{-1}$

$\Delta Gf° = -214.915 - 11.817\times10^{-3}T\ln T + 9.735\times10^{-6}T^2 + 121.850T^{-1} + 135.815\times10^{-3}T$

429.78-2000 K: $\Delta Hf° = -214.196 + 3.123\times10^{-3}T - 0.191\times10^{-6}T^2 + 112.300T^{-1}$

$\Delta Gf° = -214.196 - 3.123\times10^{-3}T\ln T + 0.191\times10^{-6}T^2 + 56.150T^{-1} + 85.885\times10^{-3}T$

Source: Data from Gurvich (95).

InF(g)
Indium Monofluoride (ideal gas)
[Formation: $In(c,l) + 0.5F_2(g) = InF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.162	56.438	56.438	0	-46.300	-51.785	37.959
300	8.169	56.489	56.439	.015	-46.304	-51.819	37.750
400	8.473	58.884	56.761	.849	-46.519	-53.627	29.300
429.78	8.525	59.494	56.930	1.102	-46.593	-54.153	27.537
429.78	8.525	59.494	56.930	1.102	-47.373	-54.153	27.537
500	8.649	60.796	57.384	1.706	-47.547	-55.247	24.148
600	8.760	62.383	58.090	2.576	-47.794	-56.765	20.676
700	8.835	63.740	58.801	3.457	-48.037	-58.240	18.183
800	8.890	64.923	59.494	4.343	-48.281	-59.681	16.304
900	8.932	65.973	60.157	5.234	-48.521	-61.092	14.835
1000	8.966	66.915	60.786	6.129	-48.761	-62.475	13.654
1100	8.995	67.772	61.384	7.027	-49.001	-63.836	12.683
1200	9.021	68.555	61.948	7.928	-49.240	-65.173	11.870
1300	9.045	69.278	62.485	8.831	-49.480	-66.492	11.178
1400	9.066	69.949	62.994	9.737	-49.719	-67.790	10.582
1500	9.087	70.576	63.480	10.644	-49.958	-69.074	10.064
1600	9.107	71.163	63.942	11.554	-50.196	-70.340	9.608
1700	9.126	71.715	64.382	12.466	-50.434	-71.589	9.203
1800	9.144	72.238	64.805	13.379	-50.672	-72.831	8.843
1900	9.163	72.732	65.208	14.295	-50.907	-74.053	8.518
2000	9.181	73.203	65.597	15.212	-51.144	-75.268	8.225

Phase change: 429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.805 + 0.210\times10^{-3}T - 0.627\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.805\times10^{-3}T + 0.105\times10^{-6}T^2 + 0.627\times10^{2}T^{-1} - 2.845$

Formation equations (kcal/mol):

298.15-429.78 K: $\Delta Hf^\circ = -46.773 + 1.931\times10^{-3}T - 4.744\times10^{-6}T^2 + 95.150T^{-1}$

$\Delta Gf^\circ = -46.773 - 1.931\times10^{-3}T\ln T + 4.744\times10^{-6}T^2 + 47.575T^{-1} - 7.757\times10^{-3}T$

429.78-2000 K: $\Delta Hf^\circ = -46.413 - 2.416\times10^{-3}T + 0.028\times10^{-6}T^2 + 29.450T^{-1}$

$\Delta Gf^\circ = -46.413 + 2.416\times10^{-3}T\ln T - 0.028\times10^{-6}T^2 + 14.725T^{-1} - 32.722\times10^{-3}T$

Source: Data from Gurvich (95).

$InF_2(g)$
Indium Difluoride (ideal gas)
[Formation: $In(c,l) + F_2(g) = InF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	11.815	69.723	69.723	0	-114.120	-116.344	85.282
300	11.832	69.796	69.723	.022	-114.124	-116.358	84.766
400	12.533	73.305	70.198	1.243	-114.336	-117.073	63.965
429.78	12.658	74.209	70.445	1.618	-114.407	-117.274	59.635
429.78	12.658	74.209	70.445	1.618	-115.187	-117.274	59.635
500	12.954	76.151	71.113	2.519	-115.348	-117.602	51.403
600	13.214	78.537	72.157	3.828	-115.571	-118.032	42.993
700	13.384	80.588	73.218	5.159	-115.788	-118.425	36.973
800	13.500	82.383	74.253	6.504	-116.003	-118.787	32.451
900	13.582	83.978	75.247	7.858	-116.216	-119.121	28.926
1000	13.642	85.412	76.193	9.219	-116.430	-119.434	26.102
1100	13.687	86.715	77.091	10.586	-116.644	-119.723	23.786
1200	13.721	87.907	77.944	11.956	-116.860	-119.994	21.854
1300	13.749	89.006	78.752	13.330	-117.076	-120.245	20.215
1400	13.771	90.026	79.522	14.706	-117.295	-120.481	18.808
1500	13.789	90.977	80.254	16.084	-117.515	-120.701	17.586
1600	13.803	91.867	80.953	17.463	-117.737	-120.907	16.515
1700	13.816	92.705	81.620	18.844	-117.959	-121.097	15.568
1800	13.827	93.495	82.258	20.226	-118.184	-121.278	14.725
1900	13.837	94.242	82.868	21.610	-118.408	-121.440	13.969
2000	13.846	94.952	83.455	22.994	-118.636	-121.596	13.287

Phase change: 429.78 K, melting point of In; $\Delta H°$ = 0.780 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.538 + 0.212\times10^{-3}T - 1.588\times10^{5}T^{-2}$

$H°- H°_{298} = 13.538\times10^{-3}T + 0.106\times10^{-6}T^2 + 1.588\times10^{2}T^{-1} - 4.578$

Formation equations (kcal/mol):

298.15-429.78 K: $\Delta Hf° = -114.882 + 2.410\times10^{-3}T - 4.830\times10^{-6}T^2 + 141.000T^{-1}$

$\Delta Gf° = -114.882 - 2.410\times10^{-3}T\ln T + 4.830\times10^{-6}T^2 + 70.500T^{-1} + 6.594\times10^{-3}T$

429.78-2000 K: $\Delta Hf° = -114.522 - 1.937\times10^{-3}T - 0.058\times10^{-6}T^2 + 75.300T^{-1}$

$\Delta Gf° = -114.522 + 1.937\times10^{-3}T\ln T + 0.058\times10^{-6}T^2 + 37.650T^{-1} - 18.371\times10^{-3}T$

Source: Data from Gurvich (95).

InF_3(c,l)

Indium Trifluoride

[Formation: $In(c,l) + 1.5F_2(g) = InF_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	21.988	26.291	26.291	0	-284.400	-266.453	195.313
300	22.005	26.427	26.291	.041	-284.392	-266.342	194.028
400	22.880	32.877	27.164	2.285	-283.965	-260.391	142.269
429.78	23.141	34.529	27.618	2.970	-283.844	-258.640	131.521
429.78	23.141	34.529	27.618	2.970	-284.624	-258.640	131.521
500	23.755	38.077	28.843	4.617	-284.323	-254.417	111.204
600	24.630	42.485	30.758	7.036	-283.851	-248.480	90.508
700	25.506	46.347	32.714	9.543	-283.316	-242.625	75.750
800	26.381	49.810	34.639	12.137	-282.714	-236.854	64.705
900	27.256	52.968	36.502	14.819	-282.034	-231.160	56.133
1000	28.131	55.885	38.297	17.588	-281.280	-225.549	49.293
1100	29.006	58.607	40.021	20.445	-280.447	-220.014	43.712
1200	29.882	61.169	41.677	23.390	-279.534	-214.561	39.076
1300	30.757	63.595	43.271	26.421	-278.540	-209.186	35.167
1400	31.632	65.906	44.805	29.541	-277.465	-203.891	31.828
1445	32.026	66.912	45.479	30.970	-276.958	-201.536	30.481
1445	32.027	77.500	45.479	46.270	-261.658	-201.536	30.481
1500	32.027	78.695	46.674	48.031	-261.025	-199.257	29.031
1600	32.027	80.762	48.741	51.234	-259.875	-195.176	26.659
1700	32.027	82.704	50.683	54.436	-258.730	-191.167	24.576
1800	32.027	84.534	52.512	57.639	-257.591	-187.227	22.732
1900	32.027	86.266	54.244	60.842	-256.452	-183.348	21.090
2000	32.027	87.909	55.887	64.044	-255.321	-179.533	19.618

Phase changes: 429.78 K, melting point of In; $\Delta H° = 0.780$ kcal/mol.
1445 K, melting point of InF_3; $\Delta H° = 15.300$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1445 K: $Cp° = 19.387 + 8.740\times10^{-3}T$

$H°- H°_{298} = 19.387\times10^{-3}T + 4.370\times10^{-6}T^2 - 6.169$

1445-2000 K: $Cp° = 32.027$

$H°- H°_{298} = 32.027\times10^{-3}T - 0.009$

Formation equations (kcal/mol):

298.15-429.78 K: $\Delta Hf° = -285.308 + 4.005\times10^{-3}T - 0.653\times10^{-6}T^2 - 68.050T^{-1}$

$\Delta Gf° = -285.308 - 4.005\times10^{-3}T\ln T + 0.653\times10^{-6}T^2 - 34.025T^{-1} + 86.245\times10^{-3}T$

429.78-1445 K: $\Delta Hf° = -284.948 - 0.342\times10^{-3}T + 4.119\times10^{-6}T^2 - 133.750T^{-1}$

$\Delta Gf° = -284.948 + 0.342\times10^{-3}T\ln T - 4.119\times10^{-6}T^2 - 66.875T^{-1} + 61.280\times10^{-3}T$

1445-2000 K: $\Delta Hf° = -278.788 + 12.298\times10^{-3}T - 0.251\times10^{-6}T^2 - 133.750T^{-1}$

$\Delta Gf° = -278.788 - 12.298\times10^{-3}T\ln T + 0.251\times10^{-6}T^2 - 66.875T^{-1} + 142.669\times10^{-3}T$

Source: Data from Gurvich (95).

$InF_3(g)$

Indium Trifluoride (ideal gas)

[Formation: $In(c,l) + 1.5F_2(g) = InF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	16.690	74.060	74.060	0	-205.000	-201.296	147.552
300	16.710	74.160	74.060	.030	-205.003	-201.273	146.625
400	17.810	79.140	74.740	1.760	-205.090	-200.021	109.285
429.78	18.001	80.426	75.090	2.293	-205.121	-199.642	101.520
429.78	18.001	80.426	75.090	2.293	-205.901	-199.642	101.520
500	18.450	83.190	76.030	3.580	-205.960	-198.611	86.812
600	18.840	86.600	77.533	5.440	-206.048	-197.145	71.809
700	19.090	89.520	79.034	7.340	-206.120	-195.650	61.084
800	19.260	92.090	80.515	9.260	-206.191	-194.155	53.040
900	19.390	94.360	81.927	11.190	-206.263	-192.642	46.779
1000	19.480	96.420	83.290	13.130	-206.338	-191.142	41.774
1100	19.540	98.280	84.571	15.080	-206.412	-189.619	37.673
1200	19.590	99.980	85.780	17.040	-206.484	-188.085	34.254
1300	19.630	101.550	86.935	19.000	-206.561	-186.549	31.361
1400	19.660	103.010	88.031	20.970	-206.636	-185.007	28.881
1500	19.690	104.370	89.077	22.940	-206.715	-183.460	26.730
1600	19.710	105.640	90.071	24.910	-206.799	-181.905	24.847
1700	19.730	106.840	91.028	26.880	-206.886	-180.354	23.186
1800	19.750	107.970	91.942	28.850	-206.979	-178.800	21.709

Phase change: 429.78 K, melting point of In; $\Delta H° = 0.780$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 19.364 + 0.288\times10^{-3}T - 2.454\times10^{5}T^{-2}$

$H°- H°_{298} = 19.364\times10^{-3}T + 0.144\times10^{-6}T^{2} + 2.454\times10^{2}T^{-1} - 6.609$

Formation equations (kcal/mol):

298.15-429.78 K: $\Delta Hf° = -206.348 + 3.982\times10^{-3}T - 4.879\times10^{-6}T^{2} + 177.350T^{-1}$

$\Delta Gf° = -206.348 - 3.982\times10^{-3}T\ln T + 4.879\times10^{-6}T^{2} + 88.675T^{-1} + 37.183\times10^{-3}T$

429.78-1800 K: $\Delta Hf° = -205.989 - 0.365\times10^{-3}T - 0.107\times10^{-6}T^{2} + 111.650T^{-1}$

$\Delta Gf° = -205.989 + 0.365\times10^{-3}T\ln T + 0.107\times10^{-6}T^{2} + 55.825T^{-1} + 12.217\times10^{-3}T$

Source: Data from Steiger (225).

InI(g)

Indium Monoiodide (ideal gas)

[Formation: $In(c,l) + 0.5I_2(c,l,g) = InI(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.826	63.860	63.860	0	1.800	-8.981	6.583
300	8.827	63.910	63.860	.016	1.792	-9.047	6.591
386.8	8.870	66.162	64.133	.785	1.384	-12.134	6.856
386.8	8.870	66.162	64.133	.785	-.471	-12.134	6.856
400	8.877	66.460	64.205	.902	-.572	-12.530	6.846
429.78	8.884	67.098	64.384	1.166	-.804	-13.411	6.820
429.78	8.884	67.098	64.384	1.166	-1.584	-13.411	6.820
458.4	8.890	67.667	64.567	1.421	-1.807	-14.190	6.765
458.4	8.890	67.667	64.567	1.421	-6.818	-14.190	6.765
500	8.900	68.440	64.858	1.791	-6.926	-14.853	6.492
600	8.913	70.070	65.600	2.682	-7.186	-16.417	5.980
700	8.921	71.440	66.336	3.573	-7.444	-17.933	5.599
800	8.926	72.630	67.048	4.466	-7.699	-19.412	5.303
900	8.930	73.690	67.736	5.359	-7.955	-20.868	5.067
1000	8.932	74.630	68.378	6.252	-8.209	-22.288	4.871
1100	8.934	75.480	68.985	7.145	-8.465	-23.682	4.705
1200	8.935	76.260	69.561	8.039	-8.720	-25.058	4.564
1300	8.936	76.970	70.099	8.932	-8.976	-26.403	4.439
1400	8.937	77.630	70.611	9.826	-9.234	-27.729	4.329
1500	8.938	78.250	71.104	10.719	-9.492	-29.047	4.232
1600	8.938	78.830	71.572	11.613	-9.750	-30.347	4.145
1700	8.939	79.370	72.013	12.507	-10.009	-31.622	4.065
1800	8.939	79.880	72.435	13.401	-10.269	-32.886	3.993
1900	8.940	80.360	72.836	14.295	-10.529	-34.129	3.926
2000	8.940	80.820	73.226	15.189	-10.790	-35.368	3.865

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.944 - 0.002\times10^{-3}T - 0.104\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.944\times10^{-3}T - 0.001\times10^{-6}T^2 + 0.104\times10^{2}T^{-1} - 2.701$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = 2.012 - 0.114\times10^{-3}T - 5.509\times10^{-6}T^2 + 93.100T^{-1}$

$\Delta Gf^\circ = 2.012 + 0.114\times10^{-3}T\ln T + 5.509\times10^{-6}T^2 + 46.550T^{-1} - 39.689\times10^{-3}T$

386.8-429.78 K: $\Delta Hf^\circ = 1.284 - 3.317\times10^{-3}T - 4.763\times10^{-6}T^2 + 93.100T^{-1}$

$\Delta Gf^\circ = 1.284 + 3.317\times10^{-3}T\ln T + 4.763\times10^{-6}T^2 + 46.550T^{-1} - 56.597\times10^{-3}T$

429.78-458.4 K: $\Delta Hf^\circ = 1.644 - 7.664\times10^{-3}T + 0.009\times10^{-6}T^2 + 27.400T^{-1}$

$\Delta Gf^\circ = 1.644 + 7.664\times10^{-3}T\ln T - 0.009\times10^{-6}T^2 + 13.700T^{-1} - 81.562\times10^{-3}T$

458.4-2000 K: $\Delta Hf^\circ = -5.713 - 2.494\times10^{-3}T - 0.025\times10^{-6}T^2 + 19.750T^{-1}$

$\Delta Gf^\circ = -5.713 + 2.494\times10^{-3}T\ln T + 0.025\times10^{-6}T^2 + 9.875T^{-1} - 33.831\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Other data from Grinberg (92).

$InI_2(g)$
Indium Diiodide (ideal gas)
[Formation: $In(c,l) + I_2(c,l,g) = InI_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	13.639	84.050	84.050	0	-5.600	-18.263	13.387
300	13.642	84.140	84.057	.025	-5.611	-18.343	13.363
386.8	13.742	87.629	84.489	1.215	-6.203	-21.958	12.406
386.8	13.742	87.629	84.489	1.215	-9.912	-21.958	12.406
400	13.757	88.090	84.600	1.396	-10.076	-22.366	12.220
429.78	13.773	89.078	84.876	1.806	-10.449	-23.265	11.830
429.78	13.773	89.078	84.876	1.806	-11.229	-23.265	11.830
458.4	13.789	89.961	85.160	2.201	-11.588	-24.052	11.467
458.4	13.789	89.961	85.160	2.201	-21.609	-24.052	11.467
500	13.812	91.160	85.610	2.775	-21.699	-24.268	10.607
600	13.842	93.680	86.750	4.158	-21.915	-24.761	9.019
700	13.860	95.820	87.903	5.542	-22.130	-25.223	7.875
800	13.872	97.670	89.009	6.929	-22.342	-25.648	7.007
900	13.880	99.300	90.058	8.318	-22.553	-26.043	6.324
1000	13.886	100.770	91.065	9.705	-22.766	-26.428	5.776
1100	13.890	102.090	92.005	11.094	-22.979	-26.780	5.321
1200	13.893	103.370	92.968	12.483	-23.194	-27.202	4.954
1300	13.896	104.410	93.739	13.872	-23.409	-27.434	4.612
1400	13.898	105.440	94.539	15.262	-23.626	-27.734	4.329
1500	13.900	106.400	95.299	16.652	-23.844	-28.021	4.083
1600	13.901	107.300	96.024	18.042	-24.063	-28.297	3.865
1700	13.902	108.140	96.709	19.432	-24.284	-28.549	3.670
1800	13.903	108.930	97.362	20.822	-24.506	-28.788	3.495
1900	13.904	109.690	97.999	22.213	-24.729	-29.034	3.340
2000	13.904	110.400	98.600	23.601	-24.956	-29.252	3.196

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.903 + 0.006\times10^{-3}T - 0.236\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.903\times10^{-3}T + 0.003\times10^{-6}T^2 + 0.236\times10^{2}T^{-1} - 4.225$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -4.926 - 1.594\times10^{-3}T - 6.251\times10^{-6}T^2 + 106.300T^{-1}$

$\Delta Gf^\circ = -4.926 + 1.594\times10^{-3}T\ln T + 6.251\times10^{-6}T^2 + 53.150T^{-1} - 56.278\times10^{-3}T$

386.8-429.78 K: $\Delta Hf^\circ = -6.381 - 7.998\times10^{-3}T - 4.759\times10^{-6}T^2 + 106.300T^{-1}$

$\Delta Gf^\circ = -6.381 + 7.998\times10^{-3}T\ln T + 4.759\times10^{-6}T^2 + 53.150T^{-1} - 90.093\times10^{-3}T$

429.78-458.4 K: $\Delta Hf^\circ = -6.021 - 12.345\times10^{-3}T + 0.013\times10^{-6}T^2 + 40.600T^{-1}$

$\Delta Gf^\circ = -6.021 + 12.345\times10^{-3}T\ln T - 0.013\times10^{-6}T^2 + 20.300T^{-1} - 115.058\times10^{-3}T$

458.4-2000 K: $\Delta Hf^\circ = -20.734 - 2.005\times10^{-3}T - 0.055\times10^{-6}T^2 + 25.300T^{-1}$

$\Delta Gf^\circ = -20.734 + 2.005\times10^{-3}T\ln T + 0.055\times10^{-6}T^2 + 12.650T^{-1} - 19.595\times10^{-3}T$

Source: Data from Grinberg (92).

$InI_3(g)$

Indium Triiodide (ideal gas)

[Formation: $In(c,l) + 1.5I_2(c,l,g) = InI_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.396	95.580	95.580	0	-28.800	-40.763	29.879
300	19.400	95.700	95.580	.036	-28.812	-40.836	29.749
386.8	19.575	100.653	96.184	1.728	-29.505	-44.231	24.991
386.8	19.575	100.653	96.184	1.728	-35.068	-44.231	24.991
400	19.602	101.310	96.342	1.987	-35.283	-44.541	24.336
429.78	19.711	102.722	96.736	2.572	-35.767	-45.209	22.989
429.78	19.711	102.722	96.736	2.572	-36.547	-45.209	22.989
458.4	19.816	103.972	97.154	3.125	-37.024	-45.772	21.822
458.4	19.816	103.972	97.154	3.125	-52.055	-45.772	21.822
500	19.968	105.700	97.794	3.953	-52.078	-45.198	19.756
600	19.751	109.300	99.425	5.925	-52.153	-43.819	15.961
700	19.783	112.340	101.051	7.902	-52.225	-42.419	13.244
800	19.804	114.990	102.637	9.882	-52.294	-41.017	11.205
900	19.818	117.320	104.139	11.863	-52.366	-39.601	9.616
1000	19.828	119.410	105.565	13.845	-52.436	-38.181	8.344
1100	19.836	121.300	106.910	15.829	-52.508	-36.751	7.302
1200	19.841	123.020	108.177	17.812	-52.583	-35.309	6.431
1300	19.845	124.610	109.382	19.796	-52.658	-33.869	5.694
1400	19.849	126.080	110.522	21.781	-52.736	-32.417	5.061
1500	19.852	127.460	111.615	23.767	-52.814	-30.979	4.514
1600	19.854	128.730	112.635	25.752	-52.895	-29.501	4.030
1700	19.856	129.940	113.624	27.737	-52.979	-28.048	3.606
1800	19.858	131.070	114.557	29.724	-53.063	-26.571	3.226
1900	19.860	132.150	115.461	31.710	-53.150	-25.108	2.888
2000	19.861	133.170	116.322	33.696	-53.239	-23.633	2.582

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
429.78 K, melting point of In; $\Delta H°$ = 0.780 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.862 + 0.006\times10^{-3}T - 0.416\times10^{5}T^{-2}$

$H°- H°_{298} = 19.862\times10^{-3}T + 0.003\times10^{-6}T^2 + 0.416\times10^{2}T^{-1} - 6.062$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -27.977 - 2.074\times10^{-3}T - 6.997\times10^{-6}T^2 + 124.300T^{-1}$

$\Delta Gf° = -27.977 + 2.074\times10^{-3}T\ln T + 6.997\times10^{-6}T^2 + 62.150T^{-1} - 57.484\times10^{-3}T$

386.8-429.78 K: $\Delta Hf° = -30.159 - 11.680\times10^{-3}T - 4.759\times10^{-6}T^2 + 124.300T^{-1}$

$\Delta Gf° = -30.159 + 11.680\times10^{-3}T\ln T + 4.759\times10^{-6}T^2 + 62.150T^{-1} - 108.207\times10^{-3}T$

429.78-458.4 K: $\Delta Hf° = -29.800 - 16.027\times10^{-3}T + 0.013\times10^{-6}T^2 + 58.600T^{-1}$

$\Delta Gf° = -29.800 + 16.027\times10^{-3}T\ln T - 0.013\times10^{-6}T^2 + 29.300T^{-1} - 133.172\times10^{-3}T$

458.4-2000 K: $\Delta Hf° = -51.870 - 0.517\times10^{-3}T - 0.089\times10^{-6}T^2 + 35.650T^{-1}$

$\Delta Gf° = -51.870 + 0.517\times10^{-3}T\ln T + 0.089\times10^{-6}T^2 + 17.825T^{-1} + 10.023\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Other data from Grinberg (92).

$IrBr_3(c)$
Iridium Tribromide
[Formation: $Ir(c) + 1.5Br_2(l,g) = IrBr_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	25.200	30.500	30.500	0	-42.500	-32.795	24.039
300	25.210	30.660	30.503	.047	-42.514	-32.735	23.847
332.6	25.370	33.269	30.649	.871	-42.767	-31.660	20.803
332.6	25.370	33.269	30.649	.871	-53.365	-31.660	20.803
400	25.700	37.970	31.495	2.590	-52.938	-27.305	14.919
500	26.190	43.760	33.380	5.190	-52.278	-20.968	9.165
600	26.670	48.580	35.530	7.830	-51.600	-14.775	5.382
700	27.160	52.730	37.701	10.520	-50.892	-8.696	2.715
800	27.650	56.390	39.815	13.260	-50.152	-2.719	.743

Phase change: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp^\circ = 23.753 + 4.864\times10^{-3}T$

$H^\circ - H^\circ_{298} = 23.753\times10^{-3}T + 2.432\times10^{-6}T^2 - 7.298$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -40.063 - 8.831\times10^{-3}T + 1.843\times10^{-6}T^2 + 9.600T^{-1}$

$\Delta Gf^\circ = -40.063 + 8.831\times10^{-3}T\ln T - 1.843\times10^{-6}T^2 + 4.800T^{-1} - 25.447\times10^{-3}T$

332.6-800 K: $\Delta Hf^\circ = -55.064 + 4.910\times10^{-3}T + 1.610\times10^{-6}T^2 - 37.500T^{-1}$

$\Delta Gf^\circ = -55.064 - 4.910\times10^{-3}T\ln T - 1.610\times10^{-6}T^2 - 18.750T^{-1} + 99.585\times10^{-3}T$

Source: Data based on Kolbin (135).

$IrF_6(g)$

Iridium Hexafluoride (ideal gas)

[Formation: $Ir(c) + 3F_2(g) = IrF_6(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	28.890	82.524	82.524	0	-130.000	-108.746	79.712
300	28.951	82.685	82.524	.052	-130.001	-108.611	79.122
400	31.957	91.480	83.700	3.112	-129.853	-101.502	55.458
500	33.728	98.832	86.022	6.405	-129.588	-94.448	41.283
600	34.833	105.123	88.716	9.844	-129.269	-87.466	31.859
700	35.534	110.467	91.398	13.348	-128.952	-80.485	25.128
800	32.027	115.239	94.073	16.933	-128.610	-73.575	20.099
900	36.369	119.474	96.641	20.550	-128.277	-66.689	16.194
1000	36.624	123.329	99.125	24.204	-127.948	-59.872	13.085
1100	36.813	126.870	101.524	27.881	-127.629	-53.118	10.554
1200	36.961	129.982	103.673	31.571	-127.327	-46.242	8.422
1300	37.066	132.790	105.697	35.221	-127.092	-39.345	6.614
1400	37.168	136.018	108.147	39.020	-126.737	-33.189	5.181
1500	37.240	138.419	109.939	42.720	-126.506	-26.288	3.830
1600	37.305	140.951	111.909	46.468	-126.251	-19.795	2.704
1700	37.351	142.807	113.298	50.165	-126.069	-12.489	1.606
1800	37.396	145.279	115.322	53.923	-125.854	-6.399	.777
1900	37.432	147.108	116.771	57.640	-125.699	.579	-.067
2000	37.462	149.033	118.350	61.366	-125.563	7.191	-.786

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 35.835 + 1.220\times10^{-3}T - 6.497\times10^{5}T^{-2}$

$H°- H°_{298} = 35.835\times10^{-3}T + 0.610\times10^{-6}T^{2} + 6.497\times10^{2}T^{-1} - 12.918$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -132.592 + 4.863\times10^{-3}T - 0.651\times10^{-6}T^{2} + 357.800T^{-1}$

$\Delta Gf° = -132.592 - 4.863\times10^{-3}T\ln T + 0.651\times10^{-6}T^{2} + 178.900T^{-1} + 105.481\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (253). Other data from Nagarajan (169).

KBr(c,1)

Potassium Bromide

[Formation: $K(c,1,g) + 0.5Br_2(1,g) = KBr(c,1)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.440	22.921	22.921	0	-94.120	-90.922	66.647
300	12.446	22.998	22.921	.023	-94.127	-90.902	66.221
332.6	12.561	24.288	22.993	.431	-94.255	-90.545	59.496
332.6	12.561	24.288	22.993	.431	-97.788	-90.545	59.496
336.35	12.574	24.429	23.008	.478	-97.786	-90.464	58.780
336.35	12.574	24.429	23.008	.478	-98.344	-90.464	58.780
400	12.799	26.627	23.415	1.285	-98.299	-88.978	48.615
500	13.168	29.522	24.356	2.583	-98.186	-86.660	37.879
600	13.546	31.956	25.424	3.919	-98.020	-84.369	30.731
700	13.928	34.073	26.512	5.293	-97.808	-82.110	25.636
800	14.312	35.958	27.577	6.705	-97.556	-79.884	21.823
900	14.698	37.666	28.605	8.155	-97.267	-77.693	18.866
1000	15.084	39.234	29.590	9.644	-96.949	-75.535	16.508
1007	15.111	39.339	29.657	9.750	-96.925	-75.385	16.361
1007	16.540	45.397	29.657	15.850	-90.825	-75.385	16.361
1043.7	16.540	45.989	30.221	16.457	-90.652	-74.825	15.668
1043.7	16.540	45.989	30.221	16.457	-109.690	-74.825	15.668
1100	16.540	46.858	31.051	17.388	-109.293	-72.955	14.495
1200	16.540	48.298	32.430	19.042	-108.588	-69.682	12.691
1300	16.540	49.621	33.701	20.696	-107.882	-66.468	11.174
1400	16.540	50.847	34.883	22.350	-107.178	-63.308	9.883

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
1007 K, melting point of KBr; ΔH° = 6.100 kcal/mol.
1043.7 K, boiling point of K to monatomic gas; ΔH° = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1007 K: $Cp^\circ = 11.188 + 3.888\times10^{-3}T + 0.087\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 11.188\times10^{-3}T + 1.944\times10^{-6}T^2 - 0.087\times10^{2}T^{-1} - 3.479$

1007-1400 K: $Cp^\circ = 16.540$

$H^\circ - H^\circ_{298} = 16.540\times10^{-3}T - 0.806$

KBr(c,l) - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -93.700 + 1.097\times10^{-3}T - 8.074\times10^{-6}T^2 - 8.700T^{-1}$

$\Delta Gf^\circ = -93.700 - 1.097\times10^{-3}T\ln T + 8.074\times10^{-6}T^2 - 4.350T^{-1} + 13.206\times10^{-3}T$

332.6-336.35 K: $\Delta Hf^\circ = -98.700 + 5.677\times10^{-3}T - 8.152\times10^{-6}T^2 - 24.400T^{-1}$

$\Delta Gf^\circ = -98.700 - 5.677\times10^{-3}T\ln T + 8.152\times10^{-6}T^2 - 12.200T^{-1} + 54.883\times10^{-3}T$

336.35-1007 K: $\Delta Hf^\circ = -98.697 - 0.122\times10^{-3}T + 1.800\times10^{-6}T^2 + 64.200T^{-1}$

$\Delta Gf^\circ = -98.697 + 0.122\times10^{-3}T\ln T - 1.800\times10^{-6}T^2 + 32.100T^{-1} + 24.090\times10^{-3}T$

1007-1043.7 K: $\Delta Hf^\circ = -96.024 + 5.230\times10^{-3}T - 0.144\times10^{-6}T^2 + 72.900T^{-1}$

$\Delta Gf^\circ = -96.024 - 5.230\times10^{-3}T\ln T + 0.144\times10^{-6}T^2 + 36.450T^{-1} + 56.481\times10^{-3}T$

1043.7-1400 K: $\Delta Hf^\circ = -117.627 + 7.568\times10^{-3}T - 0.150\times10^{-6}T^2 + 209.900T^{-1}$

$\Delta Gf^\circ = -117.627 - 7.568\times10^{-3}T\ln T + 0.150\times10^{-6}T^2 + 104.950T^{-1} + 93.361\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (255). Low-temperature heat capacities from Berg (12). High-temperature data for crystal based on Cooper (37), Mustajoki (164), and Leadbetter (143). Data for liquid based on heat capacities from Murgulescu (162).

KBr(g)
Potassium Bromide (ideal gas)
[Formation: $K(c,l,g) + 0.5Br_2(l,g) = KBr(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.824	59.852	59.852	0	-43.040	-50.853	37.276
300	8.827	59.906	59.853	.016	-43.054	-50.901	37.081
332.6	8.857	60.818	59.903	.304	-43.302	-51.742	33.999
332.6	8.857	60.818	59.903	.304	-46.834	-51.742	33.999
336.35	8.860	60.917	59.914	.337	-46.846	-51.797	33.656
336.35	8.860	60.917	59.914	.337	-47.404	-51.797	33.656
400	8.919	62.460	60.200	.904	-47.601	-52.612	28.746
500	8.972	64.456	60.858	1.799	-47.889	-53.831	23.529
600	9.011	66.095	61.598	2.698	-48.161	-54.993	20.031
700	9.041	67.487	62.343	3.601	-48.420	-56.112	17.519
800	9.068	68.696	63.063	4.506	-48.674	-57.194	15.624
900	9.092	69.765	63.749	5.414	-48.928	-58.243	14.143
1000	9.114	70.724	64.400	6.324	-49.189	-59.265	12.952
1043.7	9.124	71.114	64.673	6.722	-49.306	-59.702	12.501
1043.7	9.124	71.114	64.673	6.722	-68.344	-59.702	12.501
1100	9.136	71.594	65.015	7.237	-68.364	-59.235	11.769
1200	9.157	72.390	65.597	8.152	-68.398	-58.403	10.636
1300	9.178	73.124	66.149	9.068	-68.430	-57.570	9.678
1400	9.198	73.805	66.671	9.987	-68.461	-56.732	8.856
1500	9.218	74.440	67.168	10.908	-68.491	-55.893	8.143
1600	9.238	75.035	67.641	11.831	-68.521	-55.051	7.520
1700	9.257	75.596	68.092	12.756	-68.548	-54.210	6.969
1800	9.277	76.126	68.525	13.682	-68.576	-53.367	6.480
1900	9.296	76.628	68.938	14.611	-68.602	-52.519	6.041
2000	9.315	77.105	69.335	15.541	-68.630	-51.673	5.646

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
336.35 K, melting point of K; $\Delta H°$ = 0.558 kcal/mol.
1043.7 K, boiling point of K to monatomic gas; $\Delta H°$ = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.937 + 0.192\times10^{-3}T - 0.151\times10^{5}T^{-2}$

$H°- H°_{298} = 8.937\times10^{-3}T + 0.096\times10^{-6}T^2 + 0.151\times10^{2}T^{-1} - 2.724$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -41.864 - 1.154\times10^{-3}T - 9.922\times10^{-6}T^2 + 15.100T^{-1}$

$\Delta Gf° = -41.864 + 1.154\times10^{-3}T\ln T + 9.922\times10^{-6}T^2 + 7.550T^{-1} - 39.769\times10^{-3}T$

332.6-336.35 K: $\Delta Hf° = -46.865 + 3.426\times10^{-3}T - 10.000\times10^{-6}T^2 - 0.600T^{-1}$

$\Delta Gf° = -46.865 - 3.426\times10^{-3}T\ln T + 10.000\times10^{-6}T^2 - 0.300T^{-1} + 1.908\times10^{-3}T$

336.35-1043.7 K: $\Delta Hf° = -46.861 - 2.373\times10^{-3}T - 0.048\times10^{-6}T^2 + 88.000T^{-1}$

$\Delta Gf° = -46.861 + 2.373\times10^{-3}T\ln T + 0.048\times10^{-6}T^2 + 44.000T^{-1} - 28.885\times10^{-3}T$

1043.7-2000 K: $\Delta Hf° = -68.464 - 0.035\times10^{-3}T - 0.054\times10^{-6}T^2 + 225.000T^{-1}$

$\Delta Gf° = -68.464 + 0.035\times10^{-3}T\ln T + 0.054\times10^{-6}T^2 + 112.500T^{-1} + 7.994\times10^{-3}T$

Source: Data from JANAF (60).

$(KBr)_2(g)$

Dimeric Potassium Bromide (ideal gas)

[Formation: $2K(c,l,g) + Br_2(l,g) = (KBr)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	19.546	89.902	89.902	0	-129.200	-135.941	99.646
300	19.550	90.023	89.903	.036	-129.223	-135.982	99.062
332.6	19.595	92.042	90.015	.674	-129.657	-136.694	89.820
332.6	19.595	92.042	90.015	.674	-136.722	-136.694	89.820
336.35	19.601	92.262	90.039	.748	-136.739	-136.694	88.818
336.35	19.601	92.262	90.039	.748	-137.855	-136.694	88.818
400	19.689	95.669	90.672	1.999	-138.130	-136.453	74.554
500	19.754	100.071	92.127	3.972	-138.525	-135.988	59.440
600	19.790	103.676	93.761	5.949	-138.888	-135.445	49.335
700	19.812	106.728	95.401	7.929	-139.233	-134.844	42.100
800	19.826	109.375	96.986	9.911	-139.570	-134.195	36.660
900	19.835	111.710	98.494	11.894	-139.910	-133.502	32.418
1000	19.842	113.801	99.923	13.878	-140.268	-132.773	29.017
1043.7	19.844	114.650	100.522	14.745	-140.433	-132.440	27.732
1043.7	19.844	114.650	100.522	14.745	-178.509	-132.440	27.732
1100	19.847	115.692	101.271	15.863	-178.459	-129.956	25.819
1200	19.851	117.419	102.546	17.848	-178.371	-125.548	22.865
1300	19.854	119.008	103.752	19.833	-178.283	-121.151	20.367
1400	19.857	120.480	104.896	21.818	-178.198	-116.758	18.226
1500	19.859	121.850	105.981	23.804	-178.114	-112.372	16.372
1600	19.860	123.131	107.012	25.790	-178.033	-107.991	14.751
1700	19.861	124.335	107.996	27.776	-177.951	-103.619	13.321
1800	19.863	125.471	108.937	29.762	-177.874	-99.250	12.050
1900	19.863	126.545	109.835	31.749	-177.797	-94.881	10.914
2000	19.864	127.563	110.696	33.735	-177.727	-90.519	9.891

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
336.35 K, melting point of K; $\Delta H°$ = 0.558 kcal/mol.
1043.7 K, boiling point of K to monatomic gas; $\Delta H°$ = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.868 + 0.002\times10^{-3}T - 0.287\times10^{5}T^{-2}$

$H°- H°_{298} = 19.868\times10^{-3}T + 0.001\times10^{-6}T^2 + 0.287\times10^{2}T^{-1} - 6.020$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -127.421 - 0.315\times10^{-3}T - 20.035\times10^{-6}T^2 + 28.700T^{-1}$

$\Delta Gf° = -127.421 + 0.315\times10^{-3}T\ln T + 20.035\times10^{-6}T^2 + 14.350T^{-1} - 36.504\times10^{-3}T$

332.6-336.35 K: $\Delta Hf° = -137.422 + 8.846\times10^{-3}T - 20.190\times10^{-6}T^2 - 2.700T^{-1}$

$\Delta Gf° = -137.422 - 8.846\times10^{-3}T\ln T + 20.190\times10^{-6}T^2 - 1.350T^{-1} + 46.851\times10^{-3}T$

336.35-1043.7 K: $\Delta Hf° = -137.415 - 2.752\times10^{-3}T - 0.286\times10^{-6}T^2 + 174.500T^{-1}$

$\Delta Gf° = -137.415 + 2.752\times10^{-3}T\ln T + 0.286\times10^{-6}T^2 + 87.250T^{-1} - 14.736\times10^{-3}T$

1043.7-2000 K: $\Delta Hf° = -180.621 + 1.924\times10^{-3}T - 0.298\times10^{-6}T^2 + 448.500T^{-1}$

$\Delta Gf° = -180.621 - 1.924\times10^{-3}T\ln T + 0.298\times10^{-6}T^2 + 224.250T^{-1} + 59.024\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

KCl(c,l)
Potassium Chloride
[Formation: $K(c,l,g) + 0.5Cl_2(g) = KCl(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	12.277	19.729	19.729	0	-104.385	-97.714	71.626
300	12.288	19.805	19.729	.023	-104.382	-97.673	71.154
336.35	12.432	21.219	19.814	.472	-104.353	-96.862	62.937
336.35	12.432	21.219	19.814	.472	-104.911	-96.862	62.937
400	12.685	23.399	20.217	1.273	-104.861	-95.343	52.092
500	13.075	26.271	21.149	2.561	-104.743	-92.976	40.639
600	13.467	28.689	22.209	3.888	-104.576	-90.637	33.014
700	13.869	30.795	23.288	5.255	-104.365	-88.330	27.577
800	14.335	32.676	24.346	6.664	-104.111	-86.057	23.509
900	15.020	34.401	25.369	8.129	-103.803	-83.818	20.353
1000	16.243	36.040	26.354	9.686	-103.414	-81.618	17.837
1043.7	17.068	36.752	26.775	10.413	-103.202	-80.669	16.892
1043.7	17.068	36.752	26.775	10.413	-122.240	-80.669	16.892
1045	17.093	36.773	26.787	10.435	-122.230	-80.617	16.860
1045	17.543	42.755	26.787	16.686	-115.979	-80.617	16.860
1100	17.543	43.655	27.610	17.650	-115.535	-78.769	15.650
1200	17.543	45.181	29.010	19.405	-114.727	-75.461	13.743
1300	17.543	46.585	30.309	21.159	-113.920	-72.221	12.141
1400	17.543	47.885	31.519	22.913	-113.115	-69.043	10.778
1500	17.543	49.095	32.650	24.668	-112.310	-65.922	9.605

Phase changes: 336.35 K, melting point of K; $\Delta H° = 0.558$ kcal/mol.
1043.7 K, boiling point of K to monatomic gas; $\Delta H° = 19.038$ kcal/mol.
1045 K, melting point of KCl; $\Delta H° = 6.251$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1045 K: $Cp° = 9.996 + 5.670\times10^{-3}T + 0.527\times10^{5}T^{-2}$

$H°- H°_{298} = 9.996\times10^{-3}T + 2.835\times10^{-6}T^{2} - 0.527\times10^{2}T^{-1} - 3.056$

1045-1500 K: $Cp° = 17.543$

$H°- H°_{298} = 17.543\times10^{-3}T - 1.646$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = -104.799 + 4.537\times10^{-3}T - 7.277\times10^{-6}T^{2} - 86.850T^{-1}$

$\Delta Gf° = -104.799 - 4.537\times10^{-3}T\ln T + 7.277\times10^{-6}T^{2} - 43.425T^{-1} + 47.929\times10^{-3}T$

336.35-1043.7 K: $\Delta Hf° = -104.796 - 1.262\times10^{-3}T + 2.675\times10^{-6}T^{2} + 1.750T^{-1}$

$\Delta Gf° = -104.796 + 1.262\times10^{-3}T\ln T - 2.675\times10^{-6}T^{2} + 0.875T^{-1} + 17.136\times10^{-3}T$

1043.7-1045 K: $\Delta Hf° = -126.399 + 1.076\times10^{-3}T + 2.669\times10^{-6}T^{2} + 138.750T^{-1}$

$\Delta Gf° = -126.399 - 1.076\times10^{-3}T\ln T - 2.669\times10^{-6}T^{2} + 69.375T^{-1} + 54.015\times10^{-3}T$

1045-1500 K: $\Delta Hf° = -124.989 + 8.622\times10^{-3}T - 0.166\times10^{-6}T^{2} + 191.450T^{-1}$

$\Delta Gf° = -124.989 - 8.622\times10^{-3}T\ln T + 0.166\times10^{-6}T^{2} + 95.725T^{-1} + 102.144\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data from Douglas (59).

KCl(g)

Potassium Chloride (ideal gas)

[Formation: $K(c,l,g) + 0.5Cl_2(g) = KCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.723	57.116	57.116	0	-51.180	-55.656	40.797
300	8.726	57.170	57.117	.016	-51.185	-55.684	40.565
336.35	8.774	58.171	57.178	.334	-51.286	-56.224	36.532
336.35	8.774	58.171	57.178	.334	-51.844	-56.224	36.532
400	8.857	59.701	57.461	.896	-52.034	-57.036	31.163
500	8.930	61.685	58.113	1.786	-52.313	-58.253	25.462
600	8.979	63.318	58.850	2.681	-52.579	-59.416	21.642
700	9.015	64.705	59.589	3.581	-52.833	-60.536	18.900
800	9.046	65.911	60.306	4.484	-53.085	-61.620	16.834
900	9.072	66.978	60.989	5.390	-53.337	-62.671	15.218
1000	9.097	67.935	61.637	6.298	-53.597	-63.695	13.920
1043.7	9.107	68.324	61.909	6.696	-53.714	-64.133	13.429
1043.7	9.107	68.324	61.909	6.696	-72.752	-64.133	13.429
1100	9.119	68.803	62.249	7.209	-72.771	-63.668	12.649
1200	9.141	69.598	62.830	8.122	-72.805	-62.839	11.444
1300	9.162	70.330	63.378	9.037	-72.837	-62.007	10.424
1400	9.182	71.010	63.899	9.955	-72.868	-61.171	9.549
1500	9.202	71.644	64.395	10.874	-72.899	-60.334	8.791
1600	9.221	72.238	64.866	11.795	-72.930	-59.496	8.127
1700	9.240	72.798	65.317	12.718	-72.959	-58.656	7.541
1800	9.259	73.327	65.748	13.643	-72.988	-57.815	7.020
1900	9.278	73.828	66.160	14.570	-73.016	-56.970	6.553
2000	9.297	74.304	66.555	15.499	-73.046	-56.124	6.133

Phase changes: 336.35 K, melting point of K; $\Delta H°$ = 0.558 kcal/mol.

1043.7 K, boiling point of K to monatomic gas; $\Delta H°$ = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.930 + 0.188\times10^{-3}T - 0.234\times10^{5}T^{-2}$

$H°- H°_{298} = 8.930\times10^{-3}T + 0.094\times10^{-6}T^{2} + 0.234\times10^{2}T^{-1} - 2.749$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = -51.288 + 3.471\times10^{-3}T - 10.018\times10^{-6}T^{2} - 10.750T^{-1}$

$\Delta Gf° = -51.288 - 3.471\times10^{-3}T\ln T + 10.018\times10^{-6}T^{2} - 5.375T^{-1} + 2.196\times10^{-3}T$

336.35-1043.7 K: $\Delta Hf° = -51.285 - 2.328\times10^{-3}T - 0.066\times10^{-6}T^{2} + 77.850T^{-1}$

$\Delta Gf° = -51.285 + 2.328\times10^{-3}T\ln T + 0.066\times10^{-6}T^{2} + 38.925T^{-1} - 28.597\times10^{-3}T$

1043.7-2000 K: $\Delta Hf° = -72.888 + 0.010\times10^{-3}T - 0.072\times10^{-6}T^{2} + 214.850T^{-1}$

$\Delta Gf° = -72.888 - 0.010\times10^{-3}T\ln T + 0.072\times10^{-6}T^{2} + 107.425T^{-1} + 8.282\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data from JANAF (60).

$(KCl)_2(g)$

Dimeric Potassium Chloride (ideal gas)

[Formation: $2K(c,l,g) + Cl_2(g) = (KCl)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.327	84.309	84.309	0	-147.620	-147.651	108.230
300	19.333	84.429	84.309	.036	-147.625	-147.651	107.562
336.35	19.417	86.645	84.444	.740	-147.760	-147.647	95.935
336.35	19.417	86.645	84.444	.740	-148.876	-147.647	95.935
400	19.564	90.027	85.072	1.982	-149.137	-147.392	80.530
500	19.673	94.405	86.515	3.945	-149.513	-146.911	64.214
600	19.733	97.998	88.140	5.915	-149.864	-146.357	53.310
700	19.770	101.043	89.770	7.891	-150.198	-145.745	45.503
800	19.793	103.684	91.348	9.869	-150.530	-145.088	39.636
900	19.810	106.017	92.851	11.849	-150.864	-144.388	35.062
1000	19.822	108.105	94.274	13.831	-151.218	-143.651	31.395
1043.7	19.825	108.953	94.871	14.697	-151.381	-143.315	30.010
1043.7	19.825	108.953	94.871	14.697	-189.457	-143.315	30.010
1100	19.830	109.994	95.619	15.813	-189.407	-140.828	27.980
1200	19.837	111.720	96.889	17.797	-189.317	-136.414	24.844
1300	19.842	113.308	98.092	19.781	-189.227	-132.009	22.192
1400	19.846	114.779	99.233	21.765	-189.141	-127.610	19.921
1500	19.849	116.148	100.315	23.750	-189.056	-123.217	17.952
1600	19.852	117.429	101.345	25.735	-188.975	-118.831	16.231
1700	19.854	118.633	102.327	27.720	-188.893	-114.450	14.713
1800	19.856	119.767	103.264	29.706	-188.816	-110.073	13.365
1900	19.858	120.841	104.162	31.691	-188.741	-105.700	12.158
2000	19.859	121.860	105.021	33.677	-188.672	-101.332	11.073

Phase changes: 336.35 K, melting point of K; $\Delta H°$ = 0.558 kcal/mol.
1043.7 K, boiling point of K to monatomic gas; $\Delta H°$ = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.862 + 0.006\times10^{-3}T - 0.477\times10^{5}T^{-2}$

$H°- H°_{298} = 19.862\times10^{-3}T + 0.003\times10^{-6}T^{2} + 0.477\times10^{2}T^{-1} - 6.082$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf° = -148.420 + 8.943\times10^{-3}T - 20.221\times10^{-6}T^{2} - 20.600T^{-1}$

$\Delta Gf° = -148.420 - 8.943\times10^{-3}T\ln T + 20.221\times10^{-6}T^{2} - 10.300T^{-1} + 47.618\times10^{-3}T$

336.35-1043.7 K: $\Delta Hf° = -148.413 - 2.655\times10^{-3}T - 0.317\times10^{-6}T^{2} + 156.600T^{-1}$

$\Delta Gf° = -148.413 + 2.655\times10^{-3}T\ln T + 0.317\times10^{-6}T^{2} + 78.300T^{-1} - 13.968\times10^{-3}T$

1043.7-2000 K: $\Delta Hf° = -191.619 + 2.021\times10^{-3}T - 0.329\times10^{-6}T^{2} + 430.600T^{-1}$

$\Delta Gf° = -191.619 - 2.021\times10^{-3}T\ln T + 0.329\times10^{-6}T^{2} + 215.300T^{-1} + 59.791\times10^{-3}T$

Source: Data from JANAF (60).

KF(c,1)

Potassium Fluoride

[Formation: $K(c,1,g) + 0.5F_2(g) = KF(c,1)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	11.750	15.910	15.910	0	-135.580	-128.493	94.187
300	11.763	15.983	15.910	.022	-135.578	-128.449	93.574
336.35	11.985	17.341	15.992	.454	-135.555	-127.587	82.901
336.35	11.985	17.341	15.992	.454	-136.113	-127.587	82.901
400	12.373	19.454	16.379	1.230	-136.069	-125.977	68.830
500	12.864	22.269	17.285	2.492	-135.951	-123.468	53.967
600	13.286	24.653	18.320	3.800	-135.785	-120.986	44.068
700	13.654	26.729	19.375	5.148	-135.577	-118.534	37.008
800	13.976	28.574	20.411	6.530	-135.338	-116.117	31.721
900	14.254	30.237	21.413	7.942	-135.073	-113.729	27.617
1000	14.492	31.751	22.372	9.379	-134.797	-111.373	24.340
1043.7	14.578	32.373	22.778	10.014	-134.674	-110.352	23.107
1043.7	14.578	32.373	22.778	10.014	-153.712	-110.352	23.107
1100	14.689	33.142	23.288	10.839	-153.417	-108.020	21.461
1130	14.740	33.538	23.555	11.280	-153.258	-106.785	20.653
1130	14.882	39.763	23.555	18.315	-146.223	-106.785	20.653
1200	15.086	40.664	24.527	19.364	-145.835	-104.352	19.005
1300	15.378	41.883	25.816	20.887	-145.255	-100.919	16.966
1400	15.669	43.033	27.005	22.439	-144.650	-97.530	15.225
1500	15.960	44.124	28.110	24.021	-144.017	-94.186	13.723

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
1043.7 K, boiling point of K to monatomic gas; ΔH° = 19.038 kcal/mol.
1130 K, melting point of KF; ΔH° = 7.035 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1130 K: $Cp^\circ = 11.755 + 2.842\times10^{-3}T - 0.758\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 11.755\times10^{-3}T + 1.421\times10^{-6}T^2 + 0.758\times10^{2}T^{-1} - 3.885$

1130-1500 K: $Cp^\circ = 11.590 + 2.914\times10^{-3}T$

$H^\circ - H^\circ_{298} = 11.590\times10^{-3}T + 1.457\times10^{-6}T^2 + 3.358$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf^\circ = -136.814 + 6.455\times10^{-3}T - 8.734\times10^{-6}T^2 + 25.550T^{-1}$

$\Delta Gf^\circ = -136.814 - 6.455\times10^{-3}T\ln T + 8.734\times10^{-6}T^2 + 12.775T^{-1} + 61.937\times10^{-3}T$

336.35-1043.7 K: $\Delta Hf^\circ = -136.811 + 0.656\times10^{-3}T + 1.218\times10^{-6}T^2 + 114.150T^{-1}$

$\Delta Gf^\circ = -136.811 - 0.656\times10^{-3}T\ln T - 1.218\times10^{-6}T^2 + 57.075T^{-1} + 31.144\times10^{-3}T$

1043.7-1130 K: $\Delta Hf^\circ = -158.414 + 2.994\times10^{-3}T + 1.212\times10^{-6}T^2 + 251.150T^{-1}$

$\Delta Gf^\circ = -158.414 - 2.994\times10^{-3}T\ln T - 1.212\times10^{-6}T^2 + 125.575T^{-1} + 68.023\times10^{-3}T$

1130-1500 K: $\Delta Hf^\circ = -151.171 + 2.829\times10^{-3}T + 1.248\times10^{-6}T^2 + 175.350T^{-1}$

$\Delta Gf^\circ = -151.171 - 2.829\times10^{-3}T\ln T - 1.248\times10^{-6}T^2 + 87.675T^{-1} + 60.524\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Low-temperature heat capacities and entropy at 298 K from Westrum (263). High-temperature data based on Westrum (263) (to 530 K) and Macleod (149).

KF(g)

Potassium Fluoride (ideal gas)

[Formation: $K(c,l,g) + 0.5F_2(g) = KF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.420	54.135	54.135	0	-77.780	-82.090	60.173
300	8.426	54.187	54.135	.016	-77.784	-82.116	59.821
336.35	8.512	55.156	54.193	.324	-77.885	-82.636	53.693
336.35	8.512	55.156	54.193	.324	-78.443	-82.636	53.693
400	8.662	56.647	54.469	.871	-78.627	-83.413	45.574
500	8.794	58.595	55.105	1.745	-78.898	-84.578	36.968
600	8.877	60.206	55.826	2.628	-79.157	-85.690	31.212
700	8.935	61.579	56.552	3.519	-79.406	-86.758	27.087
800	8.979	62.775	57.256	4.415	-79.652	-87.792	23.983
900	9.015	63.835	57.929	5.315	-79.900	-88.794	21.562
1000	9.045	64.786	58.568	6.218	-80.158	-89.770	19.619
1043.7	9.057	65.173	58.837	6.614	-80.275	-90.186	18.885
1043.7	9.057	65.173	58.837	6.614	-99.313	-90.186	18.885
1100	9.072	65.650	59.174	7.124	-99.332	-89.694	17.820
1200	9.096	66.440	59.747	8.032	-99.367	-88.816	16.175
1300	9.119	67.169	60.290	8.943	-99.399	-87.934	14.783
1400	9.140	67.846	60.806	9.856	-99.433	-87.051	13.589
1500	9.161	68.477	61.296	10.771	-99.467	-86.165	12.554
1600	9.181	69.069	61.764	11.688	-99.501	-85.278	11.648
1700	9.200	69.626	62.210	12.607	-99.533	-84.388	10.849
1800	9.218	70.152	62.636	13.528	-99.566	-83.496	10.138
1900	9.237	70.651	63.045	14.451	-99.599	-82.602	9.501
2000	9.255	71.126	63.438	15.375	-99.634	-81.708	8.929

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
1043.7 K, boiling point of K to monatomic gas; ΔH° = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.895 + 0.190\times10^{-3}T - 0.473\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.895\times10^{-3}T + 0.095\times10^{-6}T^2 + 0.473\times10^{2}T^{-1} - 2.819$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf^\circ = -77.948 + 3.595\times10^{-3}T - 10.060\times10^{-6}T^2 - 2.950T^{-1}$

$\Delta Gf^\circ = -77.948 - 3.595\times10^{-3}T\ln T + 10.060\times10^{-6}T^2 - 1.475T^{-1} + 3.606\times10^{-3}T$

336.35-1043.7 K: $\Delta Hf^\circ = -77.944 - 2.204\times10^{-3}T - 0.108\times10^{-6}T^2 + 85.650T^{-1}$

$\Delta Gf^\circ = -77.944 + 2.204\times10^{-3}T\ln T + 0.108\times10^{-6}T^2 + 42.825T^{-1} - 27.187\times10^{-3}T$

1043.7-2000 K: $\Delta Hf^\circ = -99.547 + 0.134\times10^{-3}T - 0.114\times10^{-6}T^2 + 222.650T^{-1}$

$\Delta Gf^\circ = -99.547 - 0.134\times10^{-3}T\ln T + 0.114\times10^{-6}T^2 + 111.325T^{-1} + 9.692\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data from JANAF (60).

$(KF)_2(g)$

Dimeric Potassium Fluoride (ideal gas)

[Formation: $2K(c,l,g) + F_2(g) = (KF)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	18.768	76.444	76.444	0	-206.200	-205.331	150.510
300	18.780	76.560	76.444	.035	-206.205	-205.326	149.578
336.35	18.947	78.717	76.575	.721	-206.336	-205.212	133.339
336.35	18.947	78.717	76.575	.721	-207.452	-205.212	133.339
400	19.240	82.035	77.188	1.939	-207.698	-204.766	111.878
500	19.462	86.354	78.604	3.875	-208.052	-203.993	89.164
600	19.585	89.914	80.201	5.828	-208.381	-203.148	73.996
700	19.660	92.940	81.811	7.790	-208.699	-202.252	63.145
800	19.709	95.568	83.369	9.759	-209.016	-201.310	54.995
900	19.743	97.892	84.856	11.732	-209.338	-200.326	48.645
1000	19.767	99.973	86.266	13.707	-209.685	-199.309	43.558
1043.7	19.775	100.819	86.858	14.571	-209.845	-198.851	41.639
1043.7	19.775	100.819	86.858	14.571	-247.921	-198.851	41.639
1100	19.785	101.858	87.599	15.685	-247.867	-196.204	38.982
1200	19.799	103.580	88.860	17.664	-247.773	-191.511	34.878
1300	19.810	105.165	90.053	19.645	-247.679	-186.825	31.408
1400	19.818	106.634	91.187	21.626	-247.592	-182.148	28.434
1500	19.825	108.001	92.262	23.608	-247.507	-177.475	25.858
1600	19.831	109.281	93.287	25.591	-247.426	-172.810	23.604
1700	19.835	110.483	94.263	27.574	-247.345	-168.149	21.617
1800	19.839	111.617	95.196	29.558	-247.271	-163.494	19.851
1900	19.843	112.690	96.089	31.542	-247.198	-158.840	18.271
2000	19.845	113.708	96.945	33.527	-247.132	-154.192	16.849

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
1043.7 K, boiling point of K to monatomic gas; ΔH° = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.836 + 0.022\times10^{-3}T - 0.955\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.836\times10^{-3}T + 0.011\times10^{-6}T^2 + 0.955\times10^{2}T^{-1} - 6.235$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf^\circ = -207.132 + 9.236\times10^{-3}T - 20.299\times10^{-6}T^2 - 5.000T^{-1}$

$\Delta Gf^\circ = -207.132 - 9.236\times10^{-3}T\ln T + 20.299\times10^{-6}T^2 - 2.500T^{-1} + 52.640\times10^{-3}T$

336.35-1043.7 K: $\Delta Hf^\circ = -207.126 - 2.362\times10^{-3}T - 0.395\times10^{-6}T^2 + 172.200T^{-1}$

$\Delta Gf^\circ = -207.126 + 2.362\times10^{-3}T\ln T + 0.395\times10^{-6}T^2 + 86.100T^{-1} - 8.947\times10^{-3}T$

1043.7-2000 K: $\Delta Hf^\circ = -250.332 + 2.314\times10^{-3}T - 0.407\times10^{-6}T^2 + 446.200T^{-1}$

$\Delta Gf^\circ = -250.332 - 2.314\times10^{-3}T\ln T + 0.407\times10^{-6}T^2 + 223.100T^{-1} + 64.812\times10^{-3}T$

Source: Data from JANAF (60) who estimated some molecular constants.

KI(c,1)

Potassium Iodide

[Formation: $K(c,l,g) + 0.5I_2(c,l,g) = KI(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	12.600	25.410	25.410	0	-78.370	-77.199	56.588
300	12.607	25.488	25.411	.023	-78.372	-77.192	56.234
336.35	12.747	26.938	25.499	.484	-78.427	-77.046	50.062
336.35	12.747	26.938	25.499	.484	-78.985	-77.046	50.062
386.8	12.940	28.733	25.804	1.133	-79.081	-76.749	43.364
386.8	12.940	28.733	25.804	1.133	-80.935	-76.749	43.364
400	12.991	29.168	25.908	1.304	-80.991	-76.605	41.854
458.4	13.205	30.952	26.440	2.069	-81.225	-75.948	36.209
458.4	13.205	30.952	26.440	2.069	-86.236	-75.948	36.209
500	13.357	32.106	26.864	2.621	-86.176	-75.016	32.789
600	13.730	34.574	27.949	3.975	-85.997	-72.800	26.517
700	14.121	36.720	29.051	5.368	-85.769	-70.617	22.047
800	14.533	38.632	30.132	6.800	-85.499	-68.471	18.705
900	14.968	40.369	31.175	8.275	-85.188	-66.361	16.114
954	15.213	41.248	31.720	9.090	-85.006	-65.237	14.945
954	16.310	47.265	31.720	14.830	-79.266	-65.237	14.945
1000	16.310	48.033	32.453	15.580	-79.057	-64.566	14.111
1043.7	16.310	48.731	33.120	16.293	-78.861	-63.936	13.388
1043.7	16.310	48.731	33.120	16.293	-97.899	-63.936	13.388
1100	16.310	49.588	33.942	17.211	-97.517	-62.115	12.341
1200	16.310	51.007	35.305	18.842	-96.837	-58.925	10.732
1300	16.310	52.312	36.564	20.473	-96.157	-55.793	9.380
1400	16.310	53.521	37.732	22.104	-95.479	-52.713	8.229

Phase changes: 336.35 K, melting point of K; $\Delta H°$ = 0.558 kcal/mol.
386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
954 K, melting point of KI; $\Delta H°$ = 5.740 kcal/mol.
1043.7 K, boiling point of K to monatomic gas; $\Delta H°$ = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-954 K: $Cp° = 11.361 + 3.964\times10^{-3}T + 0.050\times10^{5}T^{-2}$

$H°- H°_{298} = 11.361\times10^{-3}T + 1.982\times10^{-6}T^{2} - 0.050\times10^{2}T^{-1} - 3.547$

954-1400 K: $Cp° = 16.310$

$H°- H°_{298} = 16.310\times10^{-3}T - 0.730$

KI(c,1) - Continued

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf^\circ = -78.724 + 3.877\times10^{-3}T - 8.832\times10^{-6}T^2 - 5.000T^{-1}$

$\Delta Gf^\circ = -78.724 - 3.877\times10^{-3}T\ln T + 8.832\times10^{-6}T^2 - 2.500T^{-1} + 24.595\times10^{-3}T$

336.35-386.8 K: $\Delta Hf^\circ = -78.721 - 1.922\times10^{-3}T + 1.120\times10^{-6}T^2 + 83.600T^{-1}$

$\Delta Gf^\circ = -78.721 + 1.922\times10^{-3}T\ln T - 1.120\times10^{-6}T^2 + 41.800T^{-1} - 6.199\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -79.448 - 5.124\times10^{-3}T + 1.866\times10^{-6}T^2 + 83.600T^{-1}$

$\Delta Gf^\circ = -79.448 + 5.124\times10^{-3}T\ln T - 1.866\times10^{-6}T^2 + 41.800T^{-1} - 23.106\times10^{-3}T$

458.4-954 K: $\Delta Hf^\circ = -86.805 + 0.045\times10^{-3}T + 1.832\times10^{-6}T^2 + 75.950T^{-1}$

$\Delta Gf^\circ = -86.805 - 0.045\times10^{-3}T\ln T - 1.832\times10^{-6}T^2 + 37.975T^{-1} + 24.625\times10^{-3}T$

954-1043.7 K: $\Delta Hf^\circ = -83.988 + 4.994\times10^{-3}T - 0.150\times10^{-6}T^2 + 80.950T^{-1}$

$\Delta Gf^\circ = -83.988 - 4.994\times10^{-3}T\ln T + 0.150\times10^{-6}T^2 + 40.475T^{-1} + 53.732\times10^{-3}T$

1043.7-1400 K: $\Delta Hf^\circ = -105.591 + 7.332\times10^{-3}T - 0.156\times10^{-6}T^2 + 217.950T^{-1}$

$\Delta Gf^\circ = -105.591 - 7.332\times10^{-3}T\ln T + 0.156\times10^{-6}T^2 + 108.975T^{-1} + 90.612\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (255). Low-temperature heat capacities from Berg (12). High-temperature data based on Cooper (37), Dworkin (65), and Murgulescu (162).

KI(g)

Potassium Iodide (ideal gas)

[Formation: $K(c,l,g) + 0.5I_2(c,l,g) = KI(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.872	61.704	61.704	0	-30.000	-39.651	29.064
300	8.874	61.759	61.706	.016	-30.009	-39.711	28.929
336.35	8.901	62.775	61.767	.339	-30.202	-40.875	26.559
336.35	8.901	62.775	61.767	.339	-30.760	-40.875	26.559
386.8	8.938	64.023	61.981	.790	-31.053	-42.372	23.941
386.8	8.938	64.023	61.981	.790	-32.908	-42.372	23.941
400	8.948	64.323	62.053	.908	-33.017	-42.693	23.326
458.4	8.974	65.545	62.422	1.431	-33.492	-44.072	21.012
458.4	8.974	65.545	62.422	1.431	-38.503	-44.072	21.012
500	8.993	66.325	62.715	1.805	-38.622	-44.571	19.482
600	9.027	67.968	63.458	2.706	-38.896	-45.735	16.659
700	9.055	69.362	64.205	3.610	-39.157	-46.855	14.628
800	9.081	70.572	64.926	4.517	-39.412	-47.936	13.095
900	9.104	71.643	65.614	5.426	-39.667	-48.987	11.895
1000	9.127	72.604	66.266	6.338	-39.929	-50.008	10.929
1043.7	9.136	72.995	66.540	6.737	-40.047	-50.446	10.563
1043.7	9.136	72.995	66.540	6.737	-59.085	-50.446	10.563
1100	9.148	73.475	66.882	7.252	-59.106	-49.979	9.930
1200	9.169	74.271	67.464	8.168	-59.141	-49.146	8.951
1300	9.190	75.006	68.017	9.086	-59.174	-48.312	8.122
1400	9.211	75.688	68.541	10.006	-59.207	-47.475	7.411
1500	9.231	76.324	69.039	10.928	-59.238	-46.636	6.795
1600	9.251	76.921	69.513	11.852	-59.269	-45.795	6.255
1700	9.272	77.482	69.966	12.778	-59.298	-44.953	5.779
1800	9.292	78.013	70.399	13.706	-59.328	-44.109	5.356
1900	9.312	78.516	70.813	14.636	-59.356	-43.263	4.976
2000	9.332	78.994	71.210	15.569	-59.384	-42.414	4.635

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
1043.7 K, boiling point of K to monatomic gas; ΔH° = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.937 + 0.200\times10^{-3}T - 0.111\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.937\times10^{-3}T + 0.100\times10^{-6}T^2 + 0.111\times10^{2}T^{-1} - 2.711$

KI(g) - Continued

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf^\circ = -29.518 + 1.453\times10^{-3}T - 10.714\times10^{-6}T^2 + 11.100T^{-1}$

$\Delta Gf^\circ = -29.518 - 1.453\times10^{-3}T\ln T + 10.714\times10^{-6}T^2 + 5.550T^{-1} - 28.966\times10^{-3}T$

336.35-386.8 K: $\Delta Hf^\circ = -29.515 - 4.346\times10^{-3}T - 0.762\times10^{-6}T^2 + 99.700T\text{-}1$

$\Delta Gf^\circ = -29.515 + 4.346\times10^{-3}T\ln T + 0.762\times10^{-6}T^2 + 49.850T^{-1} - 59.759\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -30.242 - 7.548\times10^{-3}T - 0.016\times10^{-6}T^2 + 99.700T\text{-}1$

$\Delta Gf^\circ = -30.242 + 7.548\times10^{-3}T\ln T + 0.016\times10^{-6}T^2 + 49.850T^{-1} - 76.667\times10^{-3}T$

458.4-1043.7 K: $\Delta Hf^\circ = -37.599 - 2.378\times10^{-3}T - 0.050\times10^{-6}T^2 + 92.050T^{-1}$

$\Delta Gf^\circ = -37.599 + 2.378\times10^{-3}T\ln T + 0.050\times10^{-6}T^2 + 46.025T^{-1} - 28.935\times10^{-3}T$

1043.7-2000 K: $\Delta Hf^\circ = -59.202 - 0.041\times10^{-3}T - 0.056\times10^{-6}T^2 + 229.050T^{-1}$

$\Delta Gf^\circ = -59.202 + 0.041\times10^{-3}T\ln T + 0.056\times10^{-6}T^2 + 114.525T^{-1} + 7.944\times10^{-3}T$

Source: Data from JANAF (60).

$(KI)_2(g)$

Dimeric Potassium Iodide (ideal gas)

[Formation: $2K(c,l,g) + I_2(c,l,g) = (KI)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	19.660	94.558	94.558	0	-100.900	-111.599	81.804
300	19.662	94.680	94.560	.036	-100.914	-111.666	81.347
336.35	19.695	96.931	94.697	.751	-101.231	-112.950	73.391
336.35	19.695	96.931	94.697	.751	-102.347	-112.950	73.391
386.8	19.741	99.688	95.171	1.747	-102.839	-114.508	64.698
386.8	19.741	99.688	95.171	1.747	-106.548	-114.508	64.698
400	19.753	100.351	95.331	2.008	-106.742	-114.776	62.710
458.4	19.778	103.045	96.148	3.162	-107.585	-115.889	55.251
458.4	19.778	103.045	96.148	3.162	-117.606	-115.889	55.251
500	19.796	104.764	96.794	3.985	-117.769	-115.725	50.582
600	19.819	108.375	98.432	5.966	-118.137	-115.280	41.990
700	19.833	111.431	100.075	7.949	-118.485	-114.775	35.834
800	19.842	114.080	101.664	9.933	-118.826	-114.222	31.204
900	19.848	116.418	103.177	11.917	-119.170	-113.627	27.592
1000	19.853	118.509	104.607	13.902	-119.532	-112.992	24.694
1043.7	19.854	119.358	105.207	14.770	-119.699	-112.701	23.599
1043.7	19.854	119.358	105.207	14.770	-157.775	-112.701	23.599
1100	19.856	120.401	105.957	15.888	-157.727	-110.271	21.909
1200	19.858	122.129	107.235	17.873	-157.645	-105.960	19.298
1300	19.860	123.719	108.443	19.859	-157.560	-101.656	17.090
1400	19.862	125.191	109.587	21.846	-157.479	-97.356	15.198
1500	19.863	126.561	110.673	23.832	-157.400	-93.065	13.559
1600	19.864	127.843	111.707	25.818	-157.324	-88.778	12.126
1700	19.865	129.047	112.691	27.805	-157.247	-84.497	10.863
1800	19.866	130.183	113.632	29.791	-157.176	-80.222	9.740
1900	19.866	131.257	114.532	31.778	-157.106	-75.948	8.736
2000	19.867	132.276	115.394	33.764	-157.042	-71.678	7.833

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 336.35 K, melting point of K; $\Delta H°$ = 0.558 kcal/mol.
386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
1043.7 K, boiling point of K to monatomic gas; $\Delta H°$ = 19.038 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.869 + 0.002\times10^{-3}T - 0.186\times10^{5}T^{-2}$

$H°- H°_{298} = 19.869\times10^{-3}T + 0.001\times10^{-6}T^2 + 0.186\times10^{2}T^{-1} - 5.986$

$(KI)_2(g)$ - Continued

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta Hf^\circ = -100.501 + 4.900\times10^{-3}T - 21.627\times10^{-6}T^2 + 18.600T^{-1}$

$\Delta Gf^\circ = -100.501 - 4.900\times10^{-3}T\ln T + 21.627\times10^{-6}T^2 + 9.300T^{-1} - 15.859\times10^{-3}T$

336.35-386.8 K: $\Delta Hf^\circ = -100.494 - 6.698\times10^{-3}T - 1.723\times10^{-6}T^2 + 195.800T^{-1}$

$\Delta Gf^\circ = -100.494 + 6.698\times10^{-3}T\ln T + 1.723\times10^{-6}T^2 + 97.900T^{-1} - 77.446\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -101.950 - 13.102\times10^{-3}T - 0.231\times10^{-6}T^2 + 195.800T^{-1}$

$\Delta Gf^\circ = -101.950 + 13.102\times10^{-3}T\ln T + 0.231\times10^{-6}T^2 + 97.900T^{-1} - 111.261\times10^{-3}T$

458.4-1043.7 K: $\Delta Hf^\circ = -116.663 - 2.762\times10^{-3}T - 0.299\times10^{-6}T^2 + 180.500T^{-1}$

$\Delta Gf^\circ = -116.663 + 2.762\times10^{-3}T\ln T + 0.299\times10^{-6}T^2 + 90.250T^{-1} - 15.798\times10^{-3}T$

1043.7-2000 K: $\Delta Hf^\circ = -159.869 + 1.914\times10^{-3}T - 0.311\times10^{-6}T^2 + 454.500T^{-1}$

$\Delta Gf^\circ = -159.869 - 1.914\times10^{-3}T\ln T + 0.311\times10^{-6}T^2 + 227.250T^{-1} + 57.961\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$LaBr_3(c,l)$

Lanthanum Tribromide

[Formation: $La(c,l) + 1.5Br_2(l,g) = LaBr_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	23.800	42.500	42.500	0	-216.800	-209.147	153.307
300	23.800	42.647	42.500	.044	-216.817	-209.099	152.326
332.6	24.126	45.119	42.638	.825	-217.130	-208.244	136.834
332.6	24.126	45.119	42.638	.825	-227.727	-208.244	136.834
400	24.800	49.635	43.447	2.475	-227.401	-204.333	111.641
500	25.500	55.245	45.263	4.991	-226.866	-198.625	86.818
550	25.850	57.701	46.283	6.280	-226.572	-195.813	77.808
550	25.850	57.701	46.283	6.280	-226.659	-195.813	77.808
600	26.200	59.965	47.330	7.581	-226.354	-193.023	70.308
700	26.900	64.061	49.435	10.238	-225.714	-187.516	58.544
800	27.500	67.693	51.493	12.960	-225.042	-182.106	49.748
900	28.100	70.969	53.479	15.741	-224.350	-176.783	42.928
1000	28.700	73.960	55.380	18.580	-223.634	-171.531	37.488
1061	29.000	75.667	56.497	20.340	-223.187	-168.363	34.680
1061	33.000	87.920	56.497	33.340	-210.187	-168.363	34.680
1100	33.000	89.112	57.633	34.627	-209.747	-166.835	33.147
1134	33.000	90.117	58.592	35.749	-209.368	-165.516	31.899
1134	33.000	90.117	58.592	35.749	-210.114	-165.516	31.899
1193	33.000	91.790	60.192	37.696	-209.525	-163.210	29.899
1193	33.000	91.790	60.192	37.696	-211.006	-163.210	29.899
1200	33.000	91.983	60.377	37.927	-210.926	-162.928	29.673
1300	33.000	94.624	62.911	41.227	-209.804	-158.982	26.727

*Data 298-1061 K estimated except enthalpy of formation at 298 K.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
550 K, α - β transition point of La; ΔH° = 0.087 kcal/mol.
1061 K, melting point of $LaBr_3$; ΔH° = 13.000 kcal/mol.
1134 K, β - γ transition point of La; ΔH° = 0.746 kcal/mol.
1193 K, melting point of La; ΔH° = 1.481 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1061 K: $Cp^\circ = 22.914 + 5.876\times10^{-3}T - 0.773\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 22.914\times10^{-3}T + 2.938\times10^{-6}T^2 + 0.773\times10^{2}T^{-1} - 7.352$

1061-1300 K: $Cp^\circ = 33.000$

$H^\circ - H^\circ_{298} = 33.000\times10^{-3}T - 1.673$

$LaBr_3$(c,l) - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -214.067 - 10.807\times10^{-3}T + 3.038\times10^{-6}T^2 + 65.300T^{-1}$

$\Delta Gf^\circ = -214.067 + 10.807\times10^{-3}T\ln T - 3.038\times10^{-6}T^2 + 32.650T^{-1} - 44.537\times10^{-3}T$

332.6-550 K: $\Delta Hf^\circ = -229.067 + 2.934\times10^{-3}T + 2.806\times10^{-6}T^2 + 18.200T^{-1}$

$\Delta Gf^\circ = -229.067 - 2.934\times10^{-3}T\ln T - 2.806\times10^{-6}T^2 + 9.100T^{-1} + 80.496\times10^{-3}T$

550-1061 K: $\Delta Hf^\circ = -230.047 + 5.200\times10^{-3}T + 1.104\times10^{-6}T^2 + 107.000T^{-1}$

$\Delta Gf^\circ = -230.047 - 5.200\times10^{-3}T\ln T - 1.104\times10^{-6}T^2 + 53.500T^{-1} + 95.493\times10^{-3}T$

1061-1134 K: $\Delta Hf^\circ = -224.368 + 15.286\times10^{-3}T - 1.835\times10^{-6}T^2 + 29.700T^{-1}$

$\Delta Gf^\circ = -224.368 - 15.286\times10^{-3}T\ln T + 1.835\times10^{-6}T^2 + 14.850T^{-1} + 157.326\times10^{-3}T$

1134-1193 K: $\Delta Hf^\circ = -221.453 + 10.130\times10^{-3}T - 0.083\times10^{-6}T^2 - 47.100T^{-1}$

$\Delta Gf^\circ = -221.453 - 10.130\times10^{-3}T\ln T + 0.083\times10^{-6}T^2 - 23.550T^{-1} + 120.507\times10^{-3}T$

1193-1300 K: $\Delta Hf^\circ = -224.455 + 11.405\times10^{-3}T - 0.083\times10^{-6}T^2 - 47.100T^{-1}$

$\Delta Gf^\circ = -224.455 - 11.405\times10^{-3}T\ln T + 0.083\times10^{-6}T^2 - 23.550T^{-1} + 132.056\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Hurtgen (103). Entropy at 298 K estimated. Other data 298-1061 K derived from estimated heat capacities. Values at 1061 K, enthalpy of fusion, and heat capacity of liquid based on Dworkin (68).

$LaBr_3(g)$
Lanthanum Tribromide (ideal gas)
[Formation: $La(c,l) + 1.5Br_2(l,g) = LaBr_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.129	91.681	91.681	0	-144.300	-151.310	110.912
300	19.138	91.799	91.682	.035	-144.326	-151.353	110.259
332.6	19.238	93.778	91.792	.661	-144.795	-152.093	99.938
332.6	19.238	93.778	91.792	.661	-155.392	-152.093	99.938
400	19.446	97.353	92.435	1.967	-155.410	-151.428	82.736
500	19.596	101.710	93.870	3.920	-155.437	-150.429	65.751
550	19.638	103.581	94.669	4.901	-155.450	-149.926	59.574
550	19.638	103.581	94.669	4.901	-155.537	-149.926	59.574
600	19.679	105.291	95.484	5.884	-155.551	-149.416	54.424
700	19.729	108.328	97.108	7.854	-155.598	-148.387	46.328
800	19.762	110.965	98.679	9.829	-155.674	-147.354	40.255
900	19.785	113.294	100.176	11.806	-155.785	-146.311	35.529
1000	19.802	115.379	101.593	13.786	-155.928	-145.244	31.743
1100	19.814	117.267	102.934	15.766	-156.108	-144.166	28.643
1134	19.817	117.870	103.373	16.440	-156.177	-143.798	27.713
1134	19.817	117.870	103.373	16.440	-156.923	-143.798	27.713
1193	19.822	118.876	104.116	17.609	-157.111	-143.110	26.216
1193	19.822	118.876	104.116	17.609	-158.592	-143.110	26.216
1200	19.823	118.992	104.202	17.748	-158.605	-143.017	26.047
1300	19.830	120.579	105.401	19.731	-158.800	-141.719	23.825
1400	19.836	122.049	106.539	21.714	-158.996	-140.394	21.916
1500	19.841	123.417	107.618	23.698	-159.194	-139.052	20.260
1600	19.844	124.698	108.647	25.682	-159.394	-137.702	18.809
1700	19.847	125.901	109.626	27.667	-159.594	-136.353	17.529
1800	19.850	127.036	110.563	29.652	-159.795	-134.977	16.388
1900	19.852	128.109	111.458	31.637	-159.998	-133.578	15.365
2000	19.854	129.127	112.316	33.622	-160.204	-132.185	14.444

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
550 K, α - β transition point of La; $\Delta H°$ = 0.087 kcal/mol.
1134 K, β - γ transition point of La; $\Delta H°$ = 0.746 kcal/mol.
1193 K, melting point of La; $\Delta H°$ = 1.481 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.844 + 0.018\times10^{-3}T - 0.640\times10^{5}T^{-2}$

$H°- H°_{298} = 19.844\times10^{-3}T + 0.009\times10^{-6}T^{2} + 0.640\times10^{2}T^{-1} - 6.132$

$LaBr_3(g)$ - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -140.347 - 13.877\times10^{-3}T + 0.109\times10^{-6}T^2 + 52.000T^{-1}$

$\Delta Gf^\circ = -140.347 + 13.877\times10^{-3}T\ln T - 0.109\times10^{-6}T^2 + 26.000T^{-1} - 116.101\times10^{-3}T$

332.6-550 K: $\Delta Hf^\circ = -155.347 - 0.136\times10^{-3}T - 0.124\times10^{-6}T^2 + 4.900T^{-1}$

$\Delta Gf^\circ = -155.347 + 0.136\times10^{-3}T\ln T + 0.124\times10^{-6}T^2 + 2.450T^{-1} + 8.932\times10^{-3}T$

550-1134 K: $\Delta Hf^\circ = -156.327 + 2.130\times10^{-3}T - 1.826\times10^{-6}T^2 + 93.700T^{-1}$

$\Delta Gf^\circ = -156.327 - 2.130\times10^{-3}T\ln T + 1.826\times10^{-6}T^2 + 46.850T^{-1} + 23.929\times10^{-3}T$

1134-1193 K: $\Delta Hf^\circ = -153.411 - 3.026\times10^{-3}T - 0.074\times10^{-6}T^2 + 16.900T^{-1}$

$\Delta Gf^\circ = -153.411 + 3.026\times10^{-3}T\ln T + 0.074\times10^{-6}T^2 + 8.450T^{-1} - 12.890\times10^{-3}T$

1193-2000 K: $\Delta Hf^\circ = -156.413 - 1.751\times10^{-3}T - 0.074\times10^{-6}T^2 + 16.900T^{-1}$

$\Delta Gf^\circ = -156.413 + 1.751\times10^{-3}T\ln T + 0.074\times10^{-6}T^2 + 8.450T^{-1} - 1.342\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

$LaCl_3(c,l)$
Lanthanum Trichloride
[Formation: $La(c,l) + 1.5Cl_2(g) = LaCl_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	23.430	32.880	32.880	0	-256.000	-237.916	174.395
300	23.456	33.025	32.882	.043	-255.992	-237.804	173.238
400*	24.701	39.955	33.818	2.455	-255.477	-231.820	126.659
500	25.696	45.577	35.625	4.976	-254.892	-225.969	98.770
550	26.141	48.048	36.643	6.273	-254.575	-223.091	88.647
550	26.141	48.048	36.643	6.273	-254.662	-223.091	88.647
600	26.586	50.342	37.690	7.591	-254.326	-220.236	80.220
700	27.413	54.503	39.800	10.292	-253.621	-214.605	67.002
800	28.194	58.215	41.875	13.072	-252.877	-209.088	57.119
900	28.936	61.578	43.879	15.929	-252.096	-203.660	49.455
1000	29.644	64.664	45.806	18.858	-251.281	-198.317	43.342
1100	30.321	67.522	47.652	21.857	-250.434	-193.061	38.357
1131	30.525	68.367	48.208	22.800	-250.166	-191.450	36.995
1131	37.700	79.861	48.208	35.800	-237.166	-191.450	36.995
1134	37.700	79.961	48.291	35.913	-237.118	-191.327	36.873
1134	37.700	79.961	48.291	35.913	-237.864	-191.327	36.873
1193	37.700	81.873	49.906	38.137	-236.996	-188.930	34.610
1193	37.700	81.873	49.906	38.137	-238.477	-188.930	34.610
1200	37.700	82.094	50.093	38.401	-238.365	-188.637	34.355
1300	37.700	85.112	52.673	42.171	-236.768	-184.566	31.028
1400	37.700	87.905	55.090	45.941	-235.174	-180.606	28.194
1500	37.700	90.506	57.365	49.711	-233.583	-176.758	25.753

*Data 400-1100 K estimated.

Phase changes: 550 K, α - β transition point of La; $\Delta H°$ = 0.087 kcal/mol.
1131 K, melting point of $LaCl_3$; $\Delta H°$ = 13.000 kcal/mol.
1134 K, β - γ transition point of La; $\Delta H°$ = 0.746 kcal/mol.
1193 K, melting point of La; $\Delta H°$ = 1.481 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1131 K: $Cp° = 22.498 + 7.274\times10^{-3}T - 1.078\times10^{5}T^{-2}$
$H°- H°_{298} = 22.498\times10^{-3}T + 3.637\times10^{-6}T^{2} + 1.078\times10^{2}T^{-1} - 7.393$

1131-1500 K: $Cp° = 37.700$
$H°- H°_{298} = 37.700\times10^{-3}T - 6.839$

$LaCl_3(c,l)$ - Continued

Formation equations (kcal/mol):

298.15-550 K: $\Delta Hf^\circ = -257.082 + 2.672\times10^{-3}T + 3.455\times10^{-6}T^2 - 6.650T^{-1}$

$\Delta Gf^\circ = -257.082 - 2.672\times10^{-3}T\ln T - 3.455\times10^{-6}T^2 - 3.325T^{-1} + 80.577\times10^{-3}T$

550-1131 K: $\Delta Hf^\circ = -258.062 + 4.938\times10^{-3}T + 1.753\times10^{-6}T^2 + 82.150T^{-1}$

$\Delta Gf^\circ = -258.062 - 4.938\times10^{-3}T\ln T - 1.753\times10^{-6}T^2 + 41.075T^{-1} + 95.574\times10^{-3}T$

1131-1134 K: $\Delta Hf^\circ = -257.507 + 20.141\times10^{-3}T - 1.884\times10^{-6}T^2 - 25.650T^{-1}$

$\Delta Gf^\circ = -257.507 - 20.141\times10^{-3}T\ln T + 1.884\times10^{-6}T^2 - 12.825T^{-1} + 197.896\times10^{-3}T$

1134-1193 K: $\Delta Hf^\circ = -254.592 + 14.985\times10^{-3}T - 0.132\times10^{-6}T^2 - 102.450T^{-1}$

$\Delta Gf^\circ = -254.592 - 14.985\times10^{-3}T\ln T + 0.132\times10^{-6}T^2 - 51.225T^{-1} + 161.077\times10^{-3}T$

1193-1500 K: $\Delta Hf^\circ = -257.594 + 16.260\times10^{-3}T - 0.132\times10^{-6}T^2 - 102.450T^{-1}$

$\Delta Gf^\circ = -257.594 - 16.260\times10^{-3}T\ln T + 0.132\times10^{-6}T^2 - 51.225T^{-1} + 172.626\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (207). Low-temperature heat capacities and entropy at 298 K from Sommers (219). High-temperature data between 350 K and 1131 K based on estimated heat capacities. Values at 1131 K, enthalpy of fusion, and heat capacity of liquid from Dworkin (66).

$LaCl_3(g)$

Lanthanum Trichloride (ideal gas)

[Formation: $La(c,l) + 1.5Cl_2(g) = LaCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.744	85.210	85.210	0	-175.300	-172.818	126.677
300	18.757	85.326	85.210	.035	-175.299	-172.802	125.885
400	19.214	90.793	85.953	1.936	-175.296	-171.974	93.961
500	19.441	95.108	87.368	3.870	-175.298	-171.140	74.804
550	19.505	96.965	88.158	4.844	-175.304	-170.723	67.838
550	19.505	96.965	88.158	4.844	-175.391	-170.723	67.838
600	19.569	98.665	88.963	5.821	-175.396	-170.300	62.031
700	19.648	101.688	90.571	7.782	-175.431	-169.445	52.902
800	19.700	104.315	92.128	9.750	-175.499	-168.590	46.056
900	19.735	106.637	93.613	11.722	-175.603	-167.720	40.727
1000	19.761	108.718	95.021	13.697	-175.742	-166.832	36.461
1100	19.780	110.602	96.353	15.674	-175.917	-165.932	32.967
1134	19.785	111.204	96.789	16.347	-175.985	-165.624	31.919
1134	19.785	111.204	96.789	16.347	-176.731	-165.624	31.919
1193	19.794	112.208	97.528	17.513	-176.920	-165.042	30.234
1193	19.794	112.208	97.528	17.513	-178.401	-165.042	30.234
1200	19.795	112.324	97.614	17.652	-178.414	-164.962	30.043
1300	19.806	113.909	98.807	19.633	-178.606	-163.841	27.544
1400	19.815	115.377	99.938	21.614	-178.801	-162.694	25.397
1500	19.822	116.745	101.015	23.595	-178.999	-161.532	23.535
1600	19.828	118.024	102.038	25.578	-179.198	-160.359	21.904
1700	19.833	119.226	103.014	27.561	-179.398	-159.185	20.464
1800	19.837	120.360	103.946	29.545	-179.601	-157.989	19.182
1900	19.841	121.433	104.839	31.529	-179.805	-156.768	18.032
2000	19.844	122.450	105.693	33.513	-180.014	-155.551	16.998

Phase changes: 550 K, α - β transition point of La; $\Delta H°$ = 0.087 kcal/mol.
1134 K, β - γ transition point of La; $\Delta H°$ = 0.746 kcal/mol.
1193 K, melting point of La; $\Delta H°$ = 1.481 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.811 + 0.038\times10^{-3}T - 0.959\times10^{5}T^{-2}$

$H°- H°_{298} = 19.811\times10^{-3}T + 0.019\times10^{-6}T^2 + 0.959\times10^{2}T^{-1} - 6.230$

Formation equations (kcal/mol):

298.15-550 K: $\Delta Hf° = -175.219 - 0.014\times10^{-3}T - 0.163\times10^{-6}T^2 - 18.550T^{-1}$

$\Delta Gf° = -175.219 + 0.014\times10^{-3}T\ln T + 0.163\times10^{-6}T^2 - 9.275T^{-1} + 8.026\times10^{-3}T$

550-1134 K: $\Delta Hf° = -176.199 + 2.252\times10^{-3}T - 1.865\times10^{-6}T^2 + 70.250T^{-1}$

$\Delta Gf° = -176.199 - 2.252\times10^{-3}T\ln T + 1.865\times10^{-6}T^2 + 35.125T^{-1} + 23.023\times10^{-3}T$

1134-1193 K: $\Delta Hf° = -173.283 - 2.904\times10^{-3}T - 0.113\times10^{-6}T^2 - 6.550T^{-1}$

$\Delta Gf° = -173.283 + 2.904\times10^{-3}T\ln T + 0.113\times10^{-6}T^2 - 3.275T^{-1} - 13.796\times10^{-3}T$

1193-2000 K: $\Delta Hf° = -176.285 - 1.629\times10^{-3}T - 0.113\times10^{-6}T^2 - 6.550T^{-1}$

$\Delta Gf° = -176.285 + 1.629\times10^{-3}T\ln T + 0.113\times10^{-6}T^2 - 3.275T^{-1} - 2.247\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

$LaF_3(c,l)$

Lanthanum Trifluoride

[Formation: $La(c,l) + 1.5F_2(g) = LaF_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	21.580	25.570	25.570	0	-406.200	-388.104	284.484
300	21.615	25.704	25.571	.040	-406.193	-387.992	282.648
400	23.045	32.135	26.437	2.279	-405.760	-381.990	208.707
500	23.893	37.376	28.116	4.630	-405.272	-376.100	164.391
550	24.148	39.670	29.066	5.832	-405.018	-373.195	148.292
550	24.148	39.670	29.066	5.832	-405.105	-373.195	148.292
600	24.403	41.782	30.039	7.046	-404.847	-370.307	134.883
700	24.738	45.570	31.993	9.504	-404.339	-364.587	113.828
800	25.027	48.892	33.901	11.993	-403.850	-358.946	98.058
900	25.379	51.859	35.735	14.512	-403.378	-353.361	85.807
1000	25.889	54.558	37.484	17.074	-402.909	-347.824	76.016
1100	26.638	57.058	39.151	19.698	-402.421	-342.337	68.015
1134	26.997	57.874	39.700	20.610	-402.245	-340.484	65.619
1134	26.997	57.874	39.700	20.610	-402.991	-340.484	65.619
1193	27.620	59.257	40.634	22.217	-402.731	-337.240	61.780
1193	27.620	59.257	40.634	22.217	-404.212	-337.240	61.780
1200	27.694	59.419	40.743	22.411	-404.169	-336.845	61.347
1300	29.116	61.689	42.267	25.249	-403.494	-331.267	55.690
1400	30.947	63.911	43.734	28.248	-402.665	-325.741	50.850
1500	33.222	66.121	45.152	31.453	-401.635	-320.274	46.663
1600	35.963	68.350	46.533	34.908	-400.359	-314.888	43.011
1700	39.180	70.624	47.882	38.661	-398.788	-309.603	39.802
1766	41.565	72.161	48.761	41.325	-397.568	-306.162	37.888
1766*	40.000	78.956	48.761	53.325	-385.568	-306.162	37.888
1800	40.000	79.719	49.338	54.685	-384.952	-304.639	36.988
1900	40.000	81.882	50.995	58.685	-383.141	-300.214	34.532
2000	40.000	83.933	52.590	62.685	-381.337	-295.896	32.334

*Heat capacity of liquid estimated.

Phase changes: 550 K, α - β transition point of La; ΔH° = 0.087 kcal/mol.
1134 K, β - γ transition point of La; ΔH° = 0.746 kcal/mol.
1193 K, melting point of La; ΔH° = 1.481 kcal/mol.
1766 K, melting point of LaF_3; ΔH° = 12.000 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1766 K: $Cp^\circ = 17.171 + 10.428\times10^{-3}T + 1.156\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 17.171\times10^{-3}T + 5.214\times10^{-6}T^2 - 1.156\times10^{2}T^{-1} - 5.195$

1766-2000 K: $Cp^\circ = 40.000$

$H^\circ - H^\circ_{298} = 40.000\times10^{-3}T - 17.315$

LaF_3(c,1) - Continued

Formation equations (kcal/mol):

298.15-550 K: $\Delta Hf^\circ = -405.053 - 2.176\times10^{-3}T + 4.903\times10^{-6}T^2 - 278.350T^{-1}$

$\Delta Gf^\circ = -405.053 + 2.176\times10^{-3}T\ln T - 4.903\times10^{-6}T^2 - 139.175T^{-1} + 47.479\times10^{-3}T$

550-1134 K: $\Delta Hf^\circ = -406.033 + 0.090\times10^{-3}T + 3.201\times10^{-6}T^2 - 189.550T^{-1}$

$\Delta Gf^\circ = -406.033 - 0.090\times10^{-3}T\ln T - 3.201\times10^{-6}T^2 - 94.775T^{-1} + 62.476\times10^{-3}T$

1134-1193 K: $\Delta Hf^\circ = -403.118 - 5.066\times10^{-3}T + 4.953\times10^{-6}T^2 - 266.350T^{-1}$

$\Delta Gf^\circ = -403.118 + 5.066\times10^{-3}T\ln T - 4.953\times10^{-6}T^2 - 133.175T^{-1} + 25.656\times10^{-3}T$

1193-1766 K: $\Delta Hf^\circ = -406.120 - 3.791\times10^{-3}T + 4.953\times10^{-6}T^2 - 266.350T^{-1}$

$\Delta Gf^\circ = -406.120 + 3.791\times10^{-3}T\ln T - 4.953\times10^{-6}T^2 - 133.175T^{-1} + 37.205\times10^{-3}T$

1766-2000 K: $\Delta Hf^\circ = -418.240 + 19.038\times10^{-3}T - 0.261\times10^{-6}T^2 - 150.750T^{-1}$

$\Delta Gf^\circ = -418.240 - 19.038\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 - 75.375T^{-1} + 205.522\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Johnson (111). Low-temperature heat capacities and entropy at 298 K from Lyon (147). High-temperature data based on Lyon (147) and Spedding 233). Heat capacity of liquid estimated.

$LaF_3(g)$

Lanthanum Trifluoride (ideal gas)

[Formation: $La(c,l) + 1.5F_2(g) = LaF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	17.379	76.900	76.900	0	-302.200	-299.408	219.469
300	17.402	77.007	76.900	.032	-302.201	-299.391	218.103
400	18.316	82.153	77.595	1.823	-302.216	-298.453	163.065
500	18.819	86.299	78.935	3.682	-302.220	-297.509	130.040
550	18.969	88.102	79.688	4.628	-302.223	-297.037	118.030
550	18.969	88.102	79.688	4.628	-302.310	-297.037	118.030
600	19.118	89.759	80.459	5.580	-302.313	-296.559	108.020
700	19.307	92.721	82.004	7.502	-302.340	-295.595	92.288
800	19.434	95.308	83.509	9.439	-302.405	-294.633	80.489
900	19.523	97.603	84.950	11.388	-302.502	-293.655	71.308
1000	19.588	99.663	86.320	13.343	-302.640	-292.661	63.960
1100	19.636	101.532	87.618	15.305	-302.814	-291.651	57.945
1134	19.649	102.130	88.045	15.973	-302.882	-291.307	56.141
1134	19.649	102.130	88.045	15.973	-303.628	-291.307	56.141
1193	19.670	103.127	88.766	17.132	-303.816	-290.662	53.247
1193	19.670	103.127	88.766	17.132	-305.297	-290.662	53.247
1200	19.673	103.242	88.850	17.270	-305.311	-290.574	52.920
1300	19.702	104.818	90.019	19.239	-305.504	-289.345	48.643
1400	19.725	106.279	91.129	21.210	-305.703	-288.094	44.973
1500	19.744	107.641	92.185	23.184	-305.904	-286.823	41.790
1600	19.759	108.916	93.192	25.159	-306.108	-285.543	39.003
1700	19.772	110.114	94.152	27.135	-306.314	-284.262	36.544
1800	19.783	111.244	95.070	29.113	-306.523	-282.956	34.355
1900	19.792	112.314	95.950	31.092	-306.734	-281.627	32.394
2000	19.799	113.329	96.794	33.071	-306.951	-280.303	30.630

Phase changes: 550 K, α - β transition point of La; ΔH° = 0.087 kcal/mol.
1134 K, β - γ transition point of La; ΔH° = 0.746 kcal/mol.
1193 K, melting point of La; ΔH° = 1.481 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.556 + 0.186\times10^{-3}T - 1.985\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.556\times10^{-3}T + 0.093\times10^{-6}T^2 + 1.985\times10^{2}T^{-1} - 6.505$

Formation equations (kcal/mol):

298.15-550 K: $\Delta Hf^\circ = -302.363 + 0.209\times10^{-3}T - 0.218\times10^{-6}T^2 + 35.750T^{-1}$

$\Delta Gf^\circ = -302.363 - 0.209\times10^{-3}T\ln T + 0.218\times10^{-6}T^2 + 17.875T^{-1} + 10.835\times10^{-3}T$

550-1134 K: $\Delta Hf^\circ = -303.343 + 2.475\times10^{-3}T - 1.920\times10^{-6}T^2 + 124.550T^{-1}$

$\Delta Gf^\circ = -303.343 - 2.475\times10^{-3}T\ln T + 1.920\times10^{-6}T^2 + 62.275T^{-1} + 25.832\times10^{-3}T$

1134-1193 K: $\Delta Hf^\circ = -300.427 - 2.681\times10^{-3}T - 0.168\times10^{-6}T^2 + 47.750T^{-1}$

$\Delta Gf^\circ = -300.427 + 2.681\times10^{-3}T\ln T + 0.168\times10^{-6}T^2 + 23.875T^{-1} - 10.987\times10^{-3}T$

1193-2000 K: $\Delta Hf^\circ = -303.429 - 1.406\times10^{-3}T - 0.168\times10^{-6}T^2 + 47.750T^{-1}$

$\Delta Gf^\circ = -303.429 + 1.406\times10^{-3}T\ln T + 0.168\times10^{-6}T^2 + 23.875T^{-1} + 0.562\times10^{-9}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

$LaI_3(c,l)$
Lanthanum Triiodide
[Formation: $La(c,l) + 1.5I_2(c,l,g) = LaI_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	23.700	51.200	51.200	0	-159.400	-158.196	115.960
300	23.727	51.347	51.200	.044	-159.404	-158.189	115.239
386.8	24.684	57.512	51.948	2.152	-159.673	-157.807	89.163
386.8	24.684	57.512	51.948	2.152	-165.237	-157.807	89.163
400	24.830	58.343	52.146	2.479	-165.379	-157.551	86.081
458.4	25.152	61.755	53.158	3.941	-165.987	-156.361	74.547
458.4	25.152	61.755	53.158	3.941	-181.019	-156.361	74.547
500	25.381	63.950	53.966	4.992	-180.800	-154.130	67.369
550	25.540	66.378	54.985	6.266	-180.529	-151.476	60.190
550	25.540	66.378	54.985	6.266	-180.616	-151.476	60.190
600	25.699	68.607	56.029	7.547	-180.337	-148.840	54.214
700	26.042	72.593	58.117	10.133	-179.777	-143.631	44.843
800	26.656	76.106	60.150	12.765	-179.204	-138.509	37.838
900	27.780	79.304	62.103	15.481	-178.584	-133.461	32.408
1000	29.650	82.320	63.975	18.345	-177.851	-128.478	28.079
1051	30.968	83.827	64.902	19.890	-177.407	-125.971	26.195
1051	36.300	96.405	64.902	33.110	-164.187	-125.971	26.195
1100	36.300	98.059	66.342	34.889	-163.475	-124.205	24.677
1134	36.300	99.164	67.309	36.123	-162.985	-123.001	23.705
1134	36.300	99.164	67.309	36.123	-163.731	-123.001	23.705
1193	36.300	101.006	68.931	38.265	-162.954	-120.902	22.148
1193	36.300	101.006	68.931	38.265	-164.435	-120.902	22.148
1200	36.300	101.218	69.119	38.519	-164.333	-120.645	21.972
1300	36.300	104.123	71.701	42.149	-162.887	-117.069	19.681

*Entropy and heat capacity at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
550 K, α - β transition point of La; ΔH° = 0.087 kcal/mol.
1051 K, melting point of LaI_3; ΔH° = 13.220 kcal/mol.
1134 K, β - γ transition point of La; ΔH° = 0.746 kcal/mol.
1193 K, melting point of La; ΔH° = 1.481 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1051 K: $Cp^\circ = 22.071 + 6.588\times10^{-3}T - 0.296\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 22.071\times10^{-3}T + 3.294\times10^{-6}T^2 + 0.296\times10^{2}T^{-1} - 6.973$

1051-1300 K: $Cp^\circ = 36.300$
$H^\circ - H^\circ_{298} = 36.300\times10^{-3}T - 5.041$

LaI_3(c,l) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -158.407 - 3.830\times10^{-3}T + 1.006\times10^{-6}T^2 + 17.600T^{-1}$

$\Delta Gf^\circ = -158.407 + 3.830\times10^{-3}T\ln T - 1.006\times10^{-6}T^2 + 8.800T^{-1} - 20.913\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -160.589 - 13.436\times10^{-3}T + 3.244\times10^{-6}T^2 + 17.600T^{-1}$

$\Delta Gf^\circ = -160.589 + 13.436\times10^{-3}T\ln T - 3.244\times10^{-6}T^2 + 8.800T^{-1} - 71.636\times10^{-3}T$

458.4-550 K: $\Delta Hf^\circ = -182.659 + 2.074\times10^{-3}T + 3.142\times10^{-6}T^2 - 5.350T^{-1}$

$\Delta Gf^\circ = -182.659 - 2.074\times10^{-3}T\ln T - 3.142\times10^{-6}T^2 - 2.675T^{-1} + 71.559\times10^{-3}T$

550-1051 K: $\Delta Hf^\circ = -183.639 + 4.340\times10^{-3}T + 1.440\times10^{-6}T^2 + 83.450T^{-1}$

$\Delta Gf^\circ = -183.639 - 4.340\times10^{-3}T\ln T - 1.440\times10^{-6}T^2 + 41.725T^{-1} + 86.556\times10^{-3}T$

1051-1134 K: $\Delta Hf^\circ = -181.707 + 18.570\times10^{-3}T - 1.854\times10^{-6}T^2 + 53.850T^{-1}$

$\Delta Gf^\circ = -181.707 - 18.570\times10^{-3}T\ln T + 1.854\times10^{-6}T^2 + 26.925T^{-1} + 180.267\times10^{-3}T$

1134-1193 K: $\Delta Hf^\circ = -178.791 + 13.413\times10^{-3}T - 0.102\times10^{-6}T^2 - 22.950T^{-1}$

$\Delta Gf^\circ = -178.791 - 13.413\times10^{-3}T\ln T + 0.102\times10^{-6}T^2 - 11.475T^{-1} + 143.448\times10^{-3}T$

1193-1300 K: $\Delta Hf^\circ = -181.794 + 14.688\times10^{-3} - 0.102\times10^{-6}T^2 - 22.950T^{-1}$

$\Delta Gf^\circ = -181.794 - 14.688\times10^{-3}T\ln T + 0.102\times10^{-6}T^2 - 11.475T^{-1} + 154.997\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (207). Entropy and heat capacity at 298 K estimated. High-temperature data based on Dworkin (69).

$LaI_3(g)$

Lanthanum Triiodide (ideal gas)

[Formation: $La(c,l) + 1.5I_2(c,l,g) = LaI_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH_f°	ΔG_f°	
298.15	19.493	98.624	98.624	0	-92.700	-105.636	77.432
300	19.497	98.745	98.625	.036	-92.712	-105.716	77.013
386.8	19.637	103.720	99.232	1.736	-93.390	-109.396	61.810
386.8	19.637	103.720	99.232	1.736	-98.953	-109.396	61.810
400	19.658	104.379	99.391	1.995	-99.163	-109.749	59.964
458.4	19.702	107.062	100.202	3.145	-100.084	-111.226	53.028
458.4	19.702	107.062	100.202	3.145	-115.115	-111.226	53.028
500	19.734	108.775	100.845	3.965	-115.127	-110.870	48.461
550	19.755	110.657	101.652	4.953	-115.142	-110.444	43.886
550	19.755	110.657	101.652	4.953	-115.229	-110.444	43.886
600	19.776	112.377	102.475	5.941	-115.242	-110.008	40.070
700	19.801	115.427	104.113	7.920	-115.290	-109.128	34.071
800	19.818	118.072	105.696	9.901	-115.368	-108.246	29.571
900	19.829	120.407	107.204	11.883	-115.482	-107.351	26.068
1000	19.837	122.497	108.631	13.866	-115.630	-106.435	23.261
1100	19.843	124.388	109.979	15.850	-115.813	-105.506	20.962
1134	19.845	124.992	110.420	16.525	-115.884	-105.188	20.272
1134	19.845	124.992	110.420	16.525	-116.630	-105.188	20.272
1193	19.848	125.999	111.166	17.696	-116.822	-104.588	19.160
1193	19.848	125.999	111.166	17.696	-118.303	-104.588	19.160
1200	19.848	126.115	111.252	17.835	-118.317	-104.505	19.033
1300	19.851	127.703	112.457	19.820	-118.516	-103.352	17.375
1400	19.854	129.175	113.600	21.805	-118.718	-102.176	15.950
1500	19.856	130.544	114.683	23.791	-118.922	-100.981	14.713
1600	19.858	131.826	115.716	25.776	-119.128	-99.776	13.629
1700	19.860	133.030	116.699	27.762	-119.336	-98.573	12.672
1800	19.861	134.165	117.638	29.748	-119.546	-97.343	11.819
1900	19.862	135.239	118.537	31.734	-119.758	-96.092	11.053
2000	19.863	136.258	119.397	33.721	-119.971	-94.841	10.364

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
550 K, α - β transition point of La; ΔH° = 0.087 kcal/mol.
1134 K, β - γ transition point of La; ΔH° = 0.746 kcal/mol.
1193 K, melting point of La; ΔH° = 1.481 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 19.866 + 0.004\times10^{-3}T - 0.332\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.866\times10^{-3}T + 0.002\times10^{-6}T^2 + 0.332\times10^{2}T^{-1} - 6.035$

$LaI_3(g)$ - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -90.769 - 6.035\times10^{-3}T - 2.286\times10^{-6}T^2 + 21.200T^{-1}$

$\Delta Gf^\circ = -90.769 + 6.035\times10^{-3}T\ln T + 2.286\times10^{-6}T^2 + 10.600T^{-1} - 85.048\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -92.951 - 15.641\times10^{-3}T - 0.048\times10^{-6}T^2 + 21.200T^{-1}$

$\Delta Gf^\circ = -92.951 + 15.641\times10^{-3}T\ln T + 0.048\times10^{-6}T^2 + 10.600T^{-1} - 135.771\times10^{-3}T$

458.4-550 K: $\Delta Hf^\circ = -115.021 - 0.131\times10^{-3}T - 0.150\times10^{-6}T^2 - 1.750T^{-1}$

$\Delta Gf^\circ = -115.021 + 0.131\times10^{-3}T\ln T + 0.150\times10^{-6}T^2 - 0.875T^{-1} + 7.424\times10^{-3}T$

550-1134 K: $\Delta Hf^\circ = -116.001 + 2.136\times10^{-3}T - 1.852\times10^{-6}T^2 + 87.050T^{-1}$

$\Delta Gf^\circ = -116.001 - 2.136\times10^{-3}T\ln T + 1.852\times10^{-6}T^2 + 43.525T^{-1} + 22.421\times10^{-3}T$

1134-1193 K: $\Delta Hf^\circ = -113.086 - 3.021\times10^{-3}T - 0.100\times10^{-6}T^2 + 10.250T^{-1}$

$\Delta Gf^\circ = -113.086 + 3.021\times10^{-3}T\ln T + 0.100\times10^{-6}T^2 + 5.125T^{-1} - 14.398\times10^{-3}T$

1193-2000 K: $\Delta Hf^\circ = -116.088 - 1.746\times10^{-3}T - 0.100\times10^{-6}T^2 + 10.250T^{-1}$

$\Delta Gf^\circ = -116.088 + 1.746\times10^{-3}T\ln T + 0.100\times10^{-6}T^2 + 5.125T^{-1} - 2.850\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Hirayama (100). Other data based on Myers (165) and Dieke (56).

LiBr(c,l)
Lithium Bromide
[Formation: $Li(c,l) + 0.5Br_2(l,g) = LiBr(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	11.910	17.690	17.690	0	-83.942	-81.720	59.901
300	11.924	17.764	17.691	.022	-83.947	-81.706	59.522
332.6	12.106	19.003	17.760	.414	-84.046	-81.458	53.525
332.6	12.106	19.003	17.760	.414	-87.578	-81.458	53.525
400	12.482	21.279	18.167	1.245	-87.466	-80.229	43.835
453.7	12.711	22.865	18.629	1.922	-87.392	-79.264	38.182
453.7	12.711	22.865	18.629	1.922	-88.109	-79.264	38.182
500	12.908	24.110	19.080	2.515	-88.056	-78.362	34.252
600	13.388	26.505	20.123	3.829	-87.898	-76.437	27.842
700	13.980	28.611	21.188	5.196	-87.678	-74.544	23.273
800	14.711	30.524	22.236	6.630	-87.384	-72.686	19.857
823	14.900	30.943	22.474	6.970	-87.306	-72.265	19.190
823	15.600	36.071	22.474	11.190	-83.086	-72.265	19.190
900	15.600	37.467	23.699	12.391	-82.763	-71.268	17.306
1000	15.600	39.110	25.159	13.951	-82.343	-70.013	15.301
1100	15.600	40.597	26.496	15.511	-81.922	-68.800	13.669
1200	15.600	41.954	27.728	17.071	-81.502	-67.626	12.316
1300	15.600	43.203	28.871	18.631	-81.080	-66.487	11.177
1400	15.600	44.359	29.937	20.191	-80.658	-65.380	10.206

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
453.7 K, melting point of Li; $\Delta H°$ = 0.717 kcal/mol.
823 K, melting point of LiBr; $\Delta H°$ = 4.220 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-823 K: $Cp° = 10.192 + 5.448\times10^{-3}T + 0.083\times10^{5}T^{-2}$
$H°- H°_{298} = 10.192\times10^{-3}T + 2.724\times10^{-6}T^2 - 0.083\times10^{2}T^{-1} - 3.253$

823-1400 K: $Cp° = 15.600$
$H°- H°_{298} = 15.600\times10^{-3}T - 1.649$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -83.789 - 0.552\times10^{-3}T - 2.684\times10^{-6}T^2 + 74.700T^{-1}$
$\Delta Gf° = -83.789 + 0.552\times10^{-3}T\ln T + 2.684\times10^{-6}T^2 + 37.350T^{-1} + 2.573\times10^{-3}T$

332.6-453.7 K: $\Delta Hf° = -88.789 + 4.028\times10^{-3}T - 2.761\times10^{-6}T^2 + 59.000T^{-1}$
$\Delta Gf° = -88.789 - 4.028\times10^{-3}T\ln T + 2.761\times10^{-6}T^2 + 29.500T^{-1} + 44.250\times10^{-3}T$

453.7-823 K: $\Delta Hf° = -88.350 - 1.070\times10^{-3}T + 2.703\times10^{-6}T^2 + 73.300T^{-1}$
$\Delta Gf° = -88.350 + 1.070\times10^{-3}T\ln T - 2.703\times10^{-6}T^2 + 36.650T^{-1} + 14.539\times10^{-3}T$

823-1400 K: $\Delta Hf° = -86.746 + 4.338\times10^{-3}T - 0.022\times10^{-6}T^2 + 81.600T^{-1}$
$\Delta Gf° = -86.746 - 4.338\times10^{-3}T\ln T + 0.022\times10^{-6}T^2 + 40.800T^{-1} + 46.645\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Low-temperature heat capacities and entropy at 298 K from Paukov (189). High-temperature data based on relative enthalpy at 823 K, enthalpy of fusion, and heat capacity values of Dworkin as quoted by JANAF (60).

LiBr(g)

Lithium Bromide (ideal gas)

[Formation: $Li(c,l,g) + 0.5Br_2(l,g) = LiBr(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.115	53.593	53.593	0	-36.800	-45.282	33.192
300	8.122	53.643	53.593	.015	-36.813	-45.335	33.026
332.6	8.228	54.486	53.640	.281	-37.036	-46.249	30.390
332.6	8.228	54.486	53.640	.281	-40.568	-46.249	30.390
400	8.446	56.028	53.916	.845	-40.724	-47.387	25.891
453.7	8.549	57.100	54.230	1.302	-40.870	-48.274	23.254
453.7	8.549	57.100	54.230	1.302	-41.587	-48.274	23.254
500	8.637	57.935	54.535	1.700	-41.729	-48.948	21.395
600	8.758	59.521	55.238	2.570	-42.015	-50.363	18.345
700	8.842	60.878	55.949	3.450	-42.282	-51.735	16.152
800	8.903	62.063	56.640	4.338	-42.534	-53.067	14.497
900	8.951	63.114	57.303	5.230	-42.782	-54.369	13.203
1000	8.990	64.059	57.932	6.127	-43.025	-55.644	12.161
1100	9.023	64.918	58.529	7.028	-43.263	-56.894	11.304
1200	9.052	65.704	59.094	7.932	-43.499	-58.123	10.585
1300	9.078	66.430	59.632	8.838	-43.731	-59.334	9.975
1400	9.101	67.103	60.141	9.747	-43.960	-60.523	9.448
1500	9.124	67.732	60.626	10.659	-44.185	-61.699	8.989
1600	9.145	68.322	61.090	11.572	-44.408	-62.859	8.586
1638	9.153	68.537	61.260	11.920	-44.491	-63.298	8.445
1638	9.153	68.537	61.260	11.920	-79.651	-63.298	8.445
1700	9.165	68.877	61.531	12.488	-79.674	-62.676	8.057
1800	9.184	69.401	61.954	13.405	-79.710	-61.675	7.488
1900	9.202	69.898	62.359	14.324	-79.745	-60.672	6.979
2000	9.220	70.370	62.748	15.245	-79.779	-59.666	6.520

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
453.7 K, melting point of Li; $\Delta H°$ = 0.717 kcal/mol.
1638 K, boiling point of Li to monatomic gas; $\Delta H°$ = 35.160 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.789 + 0.248\times10^{-3}T - 0.665\times10^{5}T^{-2}$

$H°- H°_{298} = 8.789\times10^{-3}T + 0.124\times10^{-6}T^2 + 0.665\times10^{2}T^{-1} - 2.855$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -36.249 - 1.955\times10^{-3}T - 5.284\times10^{-6}T^2 + 149.500T^{-1}$

$\Delta Gf° = -36.249 + 1.955\times10^{-3}T\ln T + 5.284\times10^{-6}T^2 + 74.750T^{-1} - 43.857\times10^{-3}T$

332.6-453.7 K: $\Delta Hf° = -41.249 + 2.625\times10^{-3}T - 5.361\times10^{-6}T^2 + 133.800T^{-1}$

$\Delta Gf° = -41.249 - 2.625\times10^{-3}T\ln T + 5.361\times10^{-6}T^2 + 66.900T^{-1} - 2.179\times10^{-3}T$

453.7-1638 K: $\Delta Hf° = -40.809 - 2.473\times10^{-3}T + 0.102\times10^{-6}T^2 + 148.100T^{-1}$

$\Delta Gf° = -40.809 + 2.473\times10^{-3}T\ln T - 0.102\times10^{-6}T^2 + 74.050T^{-1} - 31.891\times10^{-3}T$

1638-2000 K: $\Delta Hf° = -78.275 - 0.887\times10^{-3}T + 0.118\times10^{-6}T^2 - 399.800T^{-1}$

$\Delta Gf° = -78.275 + 0.887\times10^{-3}T\ln T - 0.118\times10^{-6}T^2 - 199.900T^{-1} + 2.849\times10^{-3}T$

Source: Data from JANAF (60).

$(LiBr)_2(g)$

Dimeric Lithium Bromide (ideal gas)

[Formation: $2Li(c,l,g) + Br_2(l,g) = (LiBr)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	17.937	75.148	75.148	0	-119.700	-127.112	93.175
300	17.958	75.259	75.149	.033	-119.722	-127.158	92.634
332.6	18.211	77.125	75.253	.623	-120.112	-127.947	84.072
332.6	18.211	77.125	75.253	.623	-127.177	-127.947	84.072
400	18.735	80.545	75.862	1.873	-127.366	-128.086	69.982
453.7	18.944	82.922	76.560	2.887	-127.557	-128.176	61.742
453.7	18.944	82.922	76.560	2.887	-128.991	-128.176	61.742
500	19.125	84.772	77.236	3.768	-129.189	-128.078	55.982
600	19.346	88.281	78.794	5.692	-129.579	-127.818	46.557
700	19.482	91.274	80.368	7.634	-129.930	-127.498	39.806
800	19.571	93.881	81.897	9.587	-130.256	-127.127	34.729
900	19.634	96.190	83.360	11.547	-130.577	-126.718	30.771
1000	19.678	98.261	84.748	13.513	-130.891	-126.272	27.596
1100	19.711	100.139	86.064	15.483	-131.199	-125.795	24.993
1200	19.737	101.855	87.309	17.455	-131.506	-125.291	22.818
1300	19.757	103.435	88.489	19.430	-131.808	-124.761	20.974
1400	19.772	104.900	89.610	21.406	-132.108	-124.206	19.389
1500	19.785	106.265	90.676	23.384	-132.404	-123.633	18.013
1600	19.796	107.542	91.690	25.363	-132.696	-123.037	16.806
1638	19.799	108.007	92.063	26.115	-132.805	-122.807	16.385
1638	19.799	108.007	92.063	26.115	-203.125	-122.807	16.385
1700	19.804	108.742	92.658	27.343	-203.082	-119.765	15.397
1800	19.811	109.875	93.584	29.324	-203.006	-114.867	13.947
1900	19.818	110.946	94.469	31.306	-202.932	-109.971	12.649
2000	19.823	111.962	95.318	33.288	-202.860	-105.078	11.482

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
1638 K, boiling point of Li to monatomic gas; ΔH° = 35.160 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.745 + 0.080\times10^{-3}T - 1.628\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.745\times10^{-3}T + 0.040\times10^{-6}T^2 + 1.628\times10^{2}T^{-1} - 6.437$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -119.325 - 1.744\times10^{-3}T - 10.776\times10^{-6}T^2 + 328.800T^{-1}$

$\Delta Gf^\circ = -119.325 + 1.744\times10^{-3}T\ln T + 10.776\times10^{-6}T^2 + 164.400T^{-1} - 41.118\times10^{-3}T$

332.6-453.7 K: $\Delta Hf^\circ = -129.325 + 7.417\times10^{-3}T - 10.931\times10^{-6}T^2 + 297.400T^{-1}$

$\Delta Gf^\circ = -129.325 - 7.417\times10^{-3}T\ln T + 10.931\times10^{-6}T^2 + 148.700T^{-1} + 42.237\times10^{-3}T$

453.7-1638 K: $\Delta Hf^\circ = -128.446 - 2.779\times10^{-3}T - 0.003\times10^{-6}T^2 + 326.000T^{-1}$

$\Delta Gf^\circ = -128.446 + 2.779\times10^{-3}T\ln T + 0.003\times10^{-6}T^2 + 163.000T^{-1} - 17.186\times10^{-3}T$

1638-2000 K: $\Delta Hf^\circ = -203.378 + 0.393\times10^{-3}T + 0.029\times10^{-6}T^2 - 769.800T^{-1}$

$\Delta Gf^\circ = -203.378 - 0.393\times10^{-3}T\ln T - 0.029\times10^{-6}T^2 - 384.900T^{-1} + 52.294\times10^{-3}T$

Source: Data from JANAF (60) who estimated some molecular constants.

LiCl(c,l)
Lithium Chloride
[Formation: $Li(c,l) + 0.5Cl_2(g) = LiCl(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	11.470	14.170	14.170	0	-97.660	-91.867	67.340
300	11.483	14.241	14.171	.021	-97.658	-91.832	66.899
400	12.136	17.639	14.629	1.204	-97.510	-89.911	49.125
453.7	12.450	19.187	15.078	1.864	-97.444	-88.898	42.822
453.7	12.450	19.187	15.078	1.864	-98.161	-88.898	42.822
500	12.720	20.410	15.516	2.447	-98.112	-87.952	38.443
600	13.286	22.780	16.535	3.747	-97.960	-85.934	31.301
700	13.844	24.870	17.579	5.104	-97.742	-83.947	26.209
800	14.396	26.754	18.609	6.516	-97.465	-81.994	22.399
883	14.853	28.198	19.444	7.730	-97.193	-80.402	19.900
883	14.960	33.475	19.444	12.390	-92.533	-80.402	19.900
900	14.960	33.761	19.712	12.644	-92.473	-80.170	19.468
1000	14.960	35.337	21.197	14.140	-92.114	-78.823	17.226
1100	14.960	36.763	22.548	15.636	-91.754	-77.511	15.400
1200	14.960	38.064	23.787	17.132	-91.396	-76.232	13.883
1300	14.960	39.262	24.933	18.628	-91.037	-74.983	12.606
1400	14.960	40.370	25.996	20.124	-90.678	-73.760	11.514

Phase changes: 453.7 K, melting point of Li; $\Delta H°$ = 0.717 kcal/mol.
883 K, melting point of LiCl; $\Delta H°$ = 4.660 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-883 K: $Cp° = 10.073 + 5.440\times10^{-3}T - 0.181\times10^{5}T^{-2}$

$H°- H°_{298} = 10.073\times10^{-3}T + 2.720\times10^{-6}T^{2} + 0.181\times10^{2}T^{-1} - 3.306$

883-1400 K: $Cp° = 14.960$

$H°- H°_{298} = 14.960\times10^{-3}T - 0.820$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = -98.818 + 3.960\times10^{-3}T - 2.782\times10^{-6}T^{2} + 66.950T^{-1}$

$\Delta Gf° = -98.818 - 3.960\times10^{-3}T\ln T + 2.782\times10^{-6}T^{2} + 33.475T^{-1} + 44.672\times10^{-3}T$

453.7-883 K: $\Delta Hf° = -98.378 - 1.138\times10^{-3}T + 2.682\times10^{-6}T^{2} + 81.250T^{-1}$

$\Delta Gf° = -98.378 + 1.138\times10^{-3}T\ln T - 2.682\times10^{-6}T^{2} + 40.625T^{-1} + 14.961\times10^{-3}T$

883-1400 K: $\Delta Hf° = -95.892 + 3.750\times10^{-3}T - 0.038\times10^{-6}T^{2} + 63.150T^{-1}$

$\Delta Gf° = -95.892 - 3.750\times10^{-3}T\ln T + 0.038\times10^{-6}T^{2} + 31.575T^{-1} + 42.905\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Low-temperature heat capacities and entropy at 298 K from Shirley (212). High-temperature data based on Rodigina (200).

LiCl(g)

Lithium Chloride (ideal gas)

[Formation: $Li(c,l,g) + 0.5Cl_2(g) = LiCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	7.946	50.864	50.864	0	-46.700	-51.848	38.005
300	7.954	50.913	50.864	.015	-46.704	-51.879	37.794
400	8.312	53.255	51.183	.829	-46.926	-53.573	29.270
453.7	8.431	54.311	51.489	1.280	-47.068	-54.457	26.232
453.7	8.431	54.311	51.489	1.280	-47.785	-54.457	26.232
500	8.534	55.135	51.789	1.673	-47.926	-55.129	24.096
600	8.677	56.705	52.482	2.534	-48.213	-56.542	20.595
700	8.775	58.050	53.183	3.407	-48.479	-57.910	18.080
800	8.847	59.227	53.867	4.288	-48.733	-59.241	16.184
900	8.901	60.272	54.522	5.175	-48.982	-60.539	14.701
1000	8.945	61.212	55.144	6.068	-49.226	-61.810	13.508
1100	8.981	62.067	55.736	6.964	-49.466	-63.057	12.528
1200	9.012	62.849	56.296	7.864	-49.704	-64.282	11.707
1300	9.040	63.572	56.829	8.766	-49.939	-65.488	11.009
1400	9.064	64.243	57.334	9.672	-50.170	-66.675	10.408
1500	9.087	64.869	57.816	10.579	-50.399	-67.846	9.885
1600	9.108	65.456	58.275	11.489	-50.624	-69.001	9.425
1638	9.116	65.670	58.444	11.835	-50.708	-69.437	9.264
1638	9.116	65.670	58.444	11.835	-85.868	-69.437	9.265
1700	9.128	66.009	58.714	12.401	-85.895	-68.812	8.846
1800	9.147	66.531	59.134	13.315	-85.933	-67.806	8.233
1900	9.165	67.026	59.537	14.230	-85.972	-66.798	7.683
2000	9.182	67.497	59.923	15.148	-86.010	-65.788	7.189

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
1638 K, boiling point of Li to monatomic gas; ΔH° = 35.160 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.739 + 0.256\times10^{-3}T - 0.773\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.739\times10^{-3}T + 0.128\times10^{-6}T^2 + 0.773\times10^{2}T^{-1} - 2.876$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf^\circ = -47.428 + 2.627\times10^{-3}T - 5.374\times10^{-6}T^2 + 126.150T^{-1}$

$\Delta Gf^\circ = -47.428 - 2.627\times10^{-3}T\ln T + 5.374\times10^{-6}T^2 + 63.075T^{-1} - 2.169\times10^{-3}T$

453.7-1638 K: $\Delta Hf^\circ = -46.989 - 2.472\times10^{-3}T + 0.090\times10^{-6}T^2 + 140.450T^{-1}$

$\Delta Gf^\circ = -46.989 + 2.472\times10^{-3}T\ln T - 0.090\times10^{-6}T^2 + 70.225T^{-1} - 31.880\times10^{-3}T$

1638-2000 K: $\Delta Hf^\circ = -84.455 - 0.885\times10^{-3}T + 0.106\times10^{-6}T^2 - 407.450T^{-1}$

$\Delta Gf^\circ = -84.455 + 0.885\times10^{-3}T\ln T - 0.106\times10^{-6}T^2 - 203.725T^{-1} + 2.860\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data from JANAF (60).

$(LiCl)_2(g)$

Dimeric Lithium Chloride (ideal gas)

[Formation: $2Li(c,l,g) + Cl_2(g) = (LiCl)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	17.255	68.993	68.993	0	-141.900	-142.435	104.406
300	17.283	69.099	68.993	.032	-141.905	-142.439	103.765
400	18.316	74.231	69.686	1.818	-142.191	-142.574	77.898
453.7	18.600	76.562	70.363	2.812	-142.385	-142.617	68.699
453.7	18.600	76.562	70.363	2.812	-143.819	-142.617	68.699
500	18.844	78.381	71.023	3.679	-144.019	-142.480	62.277
600	19.146	81.845	72.545	5.580	-144.413	-142.133	51.771
700	19.333	84.812	74.092	7.504	-144.767	-141.728	44.249
800	19.456	87.402	75.597	9.444	-145.097	-141.271	38.593
900	19.542	89.699	77.039	11.394	-145.419	-140.773	34.184
1000	19.604	91.761	78.409	13.352	-145.735	-140.240	30.649
1100	19.650	93.632	79.710	15.314	-146.046	-139.676	27.751
1200	19.685	95.343	80.942	17.281	-146.355	-139.084	25.330
1300	19.713	96.920	82.112	19.251	-146.659	-138.466	23.278
1400	19.735	98.382	83.222	21.224	-146.960	-137.824	21.515
1500	19.752	99.744	84.279	23.198	-147.258	-137.162	19.984
1600	19.767	101.019	85.285	25.174	-147.552	-136.477	18.642
1638	19.772	101.483	85.656	25.925	-147.662	-136.214	18.174
1638	19.772	101.483	85.656	25.925	-217.982	-136.214	18.174
1700	19.779	102.218	86.247	27.151	-217.940	-133.115	17.113
1800	19.789	103.349	87.166	29.130	-217.866	-128.129	15.557
1900	19.797	104.419	88.046	31.109	-217.795	-123.145	14.165
2000	19.805	105.434	88.889	33.089	-217.726	-118.162	12.912

Phase changes: 453.7 K, melting point of Li; $\Delta H°$ = 0.717 kcal/mol.
1638 K, boiling point of Li to monatomic gas; $\Delta H°$ = 35.160 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.664 + 0.130\times10^{-3}T - 2.176\times10^{5}T^{-2}$

$H°- H°_{298} = 19.664\times10^{-3}T + 0.065\times10^{-6}T^{2} + 2.176\times10^{2}T^{-1} - 6.598$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = -144.203 + 7.439\times10^{-3}T - 10.939\times10^{-6}T^{2} + 315.300T^{-1}$

$\Delta Gf° = -144.203 - 7.439\times10^{-3}T\ln T + 10.939\times10^{-6}T^{2} + 157.650T^{-1} + 43.279\times10^{-3}T$

453.7-1638 K: $\Delta Hf° = -143.324 - 2.757\times10^{-3}T - 0.011\times10^{-6}T^{2} + 343.900T^{-1}$

$\Delta Gf° = -143.324 + 2.757\times10^{-3}T\ln T + 0.011\times10^{-6}T^{2} + 171.950T^{-1} - 16.144\times10^{-3}T$

1638-2000 K: $\Delta Hf° = -218.256 + 0.415\times10^{-3}T + 0.021\times10^{-6}T^{2} - 751.900T^{-1}$

$\Delta Gf° = -218.256 - 0.415\times10^{-3}T\ln T - 0.021\times10^{-6}T^{2} - 375.950T^{-1} + 53.336\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data from JANAF (60).

$(LiCl)_3(g)$

Trimeric Lithium Chloride (ideal gas)

[Formation: $3Li(c,1,g) + 1.5Cl_2(g) = (LiCl)_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	24.380	80.223	80.223	0	-230.000	-223.866	164.096
300	24.441	80.374	80.224	.045	-230.010	-223.829	163.057
400	26.976	87.786	81.216	2.628	-230.535	-221.686	121.122
453.7	27.774	91.247	82.201	4.104	-230.841	-220.484	106.207
453.7	27.774	91.247	82.201	4.104	-232.992	-220.484	106.207
500	28.462	93.979	83.167	5.406	-233.291	-219.186	95.805
600	29.376	99.255	85.420	8.301	-233.839	-216.311	78.790
700	29.969	103.831	87.731	11.270	-234.286	-213.356	66.612
800	30.372	107.861	90.000	14.289	-234.673	-210.340	57.462
900	30.657	111.456	92.188	17.341	-235.029	-207.277	50.333
1000	30.865	114.697	94.279	20.418	-235.363	-204.175	44.622
1100	31.021	117.646	96.271	23.512	-235.678	-201.041	39.943
1200	31.142	120.351	98.167	26.621	-235.983	-197.881	36.039
1300	31.236	122.848	99.971	29.740	-236.275	-194.694	32.731
1400	31.312	125.165	101.689	32.867	-236.559	-191.483	29.891
1500	31.373	127.328	103.327	36.002	-236.832	-188.255	27.428
1600	31.424	129.354	104.891	39.141	-237.098	-185.006	25.270
1638	31.440	130.092	105.467	40.335	-237.196	-183.769	24.519
1638	31.440	130.092	105.467	40.335	-342.676	-183.769	24.519
1700	31.466	131.260	106.386	42.286	-342.501	-177.749	22.851
1800	31.501	133.060	107.819	45.434	-342.210	-168.070	20.406
1900	31.531	134.764	109.192	48.586	-341.920	-158.402	18.220
2000	31.556	136.382	110.512	51.740	-341.633	-148.748	16.254

Phase changes: 453.7 K, melting point of Li; $\Delta H° = 0.717$ kcal/mol.

1638 K, boiling point of Li to monatomic gas; $\Delta H° = 35.160$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 30.329 + 0.908\times10^{-3}T - 5.529\times10^{5}T^{-2}$

$H°- H°_{298} = 30.329\times10^{-3}T + 0.454\times10^{-6}T^2 + 5.529\times10^{2}T^{-1} - 10.937$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = -234.494 + 11.992\times10^{-3}T - 16.052\times10^{-6}T^2 + 699.450T^{-1}$

$\Delta Gf° = -234.494 - 11.992\times10^{-3}T\ln T + 16.052\times10^{-6}T^2 + 349.725T^{-1} + 95.251\times10^{-3}T$

453.7-1638 K: $\Delta Hf° = -233.175 - 3.302\times10^{-3}T + 0.340\times10^{-6}T^2 + 742.350T^{-1}$

$\Delta Gf° = -233.175 + 3.302\times10^{-3}T\ln T - 0.340\times10^{-6}T^2 + 371.175T^{-1} + 6.116\times10^{-3}T$

1638-2000 K: $\Delta Hf° = -345.574 + 1.456\times10^{-3}T + 0.388\times10^{-6}T^2 - 901.350T^{-1}$

$\Delta Gf° = -345.574 - 1.456\times10^{-3}T\ln T - 0.388\times10^{-6}T^2 - 450.675T^{-1} + 110.336\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data from JANAF (60).

LiF(c,l)
Lithium Fluoride
[Formation: $Li(c,l) + 0.5F_2(g) = LiF(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	10.000	8.520	8.520	0	-147.220	-140.465	102.962
300	10.033	8.582	8.520	.019	-147.219	-140.423	102.297
400	11.205	11.652	8.932	1.088	-147.156	-138.167	75.490
453.7	11.535	13.088	9.338	1.701	-147.122	-136.964	65.975
453.7	11.535	13.088	9.338	1.701	-147.839	-136.964	65.975
500	11.819	14.223	9.739	2.242	-147.822	-135.852	59.380
600	12.274	16.419	10.674	3.447	-147.744	-133.465	48.614
700	12.706	18.344	11.635	4.696	-147.620	-131.095	40.929
800	13.171	20.070	12.584	5.989	-147.450	-128.746	35.171
900	13.697	21.651	13.504	7.332	-147.233	-126.420	30.699
1000	14.297	23.124	14.393	8.731	-146.964	-124.122	27.126
1100	14.980	24.518	15.251	10.194	-146.632	-121.852	24.210
1121.3	15.137	24.807	15.430	10.515	-146.552	-121.374	23.656
1121.3	15.380	30.573	15.430	16.980	-140.087	-121.374	23.656
1200	15.380	31.616	16.458	18.190	-139.770	-120.072	21.868
1300	15.380	32.847	17.672	19.728	-139.365	-118.447	19.912
1400	15.380	33.987	18.797	21.266	-138.962	-116.853	18.241

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
1121.3 K, melting point of LiF; ΔH° = 6.465 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1121.3 K: $Cp^\circ = 10.345 + 3.998\times10^{-3}T - 1.365\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 10.345\times10^{-3}T + 1.999\times10^{-6}T^2 + 1.365\times10^{2}T^{-1} - 3.720$

1121.3-1400 K: $Cp^\circ = 15.380$

$H^\circ - H^\circ_{298} = 15.380\times10^{-3}T - 0.266$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf^\circ = -148.782 + 4.392\times10^{-3}T - 3.546\times10^{-6}T^2 + 169.250T^{-1}$

$\Delta Gf^\circ = -148.782 - 4.392\times10^{-3}T\ln T + 3.546\times10^{-6}T^2 + 84.625T^{-1} + 50.909\times10^{-3}T$

453.7-1121.3 K: $\Delta Hf^\circ = -148.342 - 0.706\times10^{-3}T + 1.918\times10^{-6}T^2 + 183.550T^{-1}$

$\Delta Gf^\circ = -148.342 + 0.706\times10^{-3}T\ln T - 1.918\times10^{-6}T^2 + 91.775T^{-1} + 21.197\times10^{-3}T$

1121.3-1400 K: $\Delta Hf^\circ = -144.888 + 4.329\times10^{-3}T - 0.081\times10^{-6}T^2 + 47.050T^{-1}$

$\Delta Gf^\circ = -144.888 - 4.329\times10^{-3}T\ln T + 0.081\times10^{-6}T^2 + 23.525T^{-1} + 51.286\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (255). Low-temperature heat capacities from Clusius (33). High-temperature data based on Douglas (57), Voskresenskaya (251), and Macleod (149).

LiF(g)
Lithium Fluoride (ideal gas)
[Formation: $Li(c,l,g) + 0.5F_2(g) = LiF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	7.478	47.840	47.840	0	-81.220	-86.189	63.177
300	7.485	47.887	47.840	.014	-81.224	-86.220	62.810
400	7.879	50.096	48.139	.783	-81.461	-87.849	47.998
453.7	8.040	51.100	48.432	1.211	-81.613	-88.700	42.727
453.7	8.040	51.100	48.432	1.211	-82.330	-88.700	42.727
500	8.178	51.888	48.716	1.586	-82.478	-89.341	39.050
600	8.391	53.399	49.374	2.415	-82.776	-90.685	33.031
700	8.546	54.705	50.044	3.263	-83.052	-91.981	28.717
800	8.660	55.854	50.700	4.123	-83.315	-93.239	25.472
900	8.747	56.879	51.330	4.994	-83.571	-94.463	22.939
1000	8.816	57.804	51.932	5.872	-83.823	-95.660	20.906
1100	8.872	58.647	52.504	6.757	-84.069	-96.831	19.238
1200	8.919	59.421	53.049	7.646	-84.314	-97.982	17.845
1300	8.959	60.137	53.568	8.540	-84.553	-99.112	16.662
1400	8.994	60.802	54.061	9.438	-84.790	-100.222	15.645
1500	9.025	61.424	54.531	10.339	-85.024	-101.317	14.762
1600	9.052	62.007	54.980	11.243	-85.254	-102.394	13.986
1638	9.062	62.220	55.146	11.587	-85.340	-102.801	13.716
1638	9.062	62.220	55.146	11.587	-120.500	-102.801	13.716
1700	9.078	62.556	55.410	12.149	-120.530	-102.128	13.129
1800	9.102	63.076	55.822	13.058	-120.574	-101.045	12.268
1900	9.124	63.569	56.216	13.970	-120.616	-99.959	11.498
2000	9.145	64.037	56.596	14.883	-120.660	-98.869	10.804

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
1638 K, boiling point of Li to monatomic gas; ΔH° = 35.160 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.318 + 0.516\times10^{-3}T - 0.883\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.318\times10^{-3}T + 0.258\times10^{-6}T^2 + 0.883\times10^{2}T^{-1} - 2.799$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf^\circ = -81.861 + 2.365\times10^{-3}T - 5.287\times10^{-6}T^2 + 121.050T^{-1}$

$\Delta Gf^\circ = -81.861 - 2.365\times10^{-3}T\ln T + 5.287\times10^{-6}T^2 + 60.525T^{-1} - 3.296\times10^{-3}T$

453.7-1638 K: $\Delta Hf^\circ = -81.421 - 2.733\times10^{-3}T + 0.177\times10^{-6}T^2 + 135.350T^{-1}$

$\Delta Gf^\circ = -81.421 + 2.733\times10^{-3}T\ln T - 0.177\times10^{-6}T^2 + 67.675T^{-1} - 33.008\times10^{-3}T$

1638-2000 K: $\Delta Hf^\circ = -118.888 - 1.147\times10^{-3}T + 0.193\times10^{-6}T^2 - 412.550T^{-1}$

$\Delta Gf^\circ = -118.888 + 1.147\times10^{-3}T\ln T - 0.193\times10^{-6}T^2 - 206.275T^{-1} + 1.732\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data from JANAF (60).

$(LiF)_2(g)$

Dimeric Lithium Fluoride (ideal gas)

[Formation: $2Li(c,l,g) + F_2(g) = (LiF)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	15.088	61.788	61.788	0	-224.800	-224.632	164.658
300	15.130	61.881	61.788	.028	-224.808	-224.632	163.642
400	16.813	66.487	62.404	1.633	-225.214	-224.510	122.665
453.7	17.330	68.646	63.016	2.554	-225.453	-224.404	108.095
453.7	17.330	68.646	63.016	2.554	-226.887	-224.404	108.095
500	17.776	70.352	63.618	3.367	-227.120	-224.134	97.968
600	18.359	73.648	65.021	5.176	-227.567	-223.494	81.406
700	18.734	76.509	66.463	7.032	-227.959	-222.785	69.556
800	18.987	79.028	67.879	8.919	-228.318	-222.022	60.653
900	19.165	81.275	69.245	10.827	-228.663	-221.213	53.717
1000	19.295	83.301	70.551	12.750	-229.000	-220.368	48.161
1100	19.392	85.145	71.796	14.684	-229.328	-219.488	43.608
1200	19.467	86.836	72.979	16.628	-229.651	-218.581	39.809
1300	19.526	88.396	74.106	18.577	-229.969	-217.645	36.589
1400	19.572	89.845	75.179	20.532	-230.284	-216.686	33.826
1500	19.610	91.197	76.203	22.491	-230.594	-215.705	31.428
1600	19.642	92.463	77.179	24.454	-230.899	-214.699	29.326
1638	19.652	92.924	77.539	25.201	-231.013	-214.315	28.595
1638	19.652	92.924	77.539	25.201	-301.333	-214.315	28.595
1700	19.668	93.655	78.114	26.420	-301.297	-211.017	27.128
1800	19.689	94.780	79.009	28.387	-301.236	-205.710	24.976
1900	19.708	95.845	79.868	30.357	-301.175	-200.405	23.052
2000	19.724	96.856	80.692	32.329	-301.116	-195.100	21.319

Phase changes: 453.7 K, melting point of Li; $\Delta H° = 0.717$ kcal/mol.

1638 K, boiling point of Li to monatomic gas; $\Delta H° = 35.160$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.042 + 0.514\times10^{-3}T - 3.651\times10^{5}T^{-2}$

$H°- H°_{298} = 19.042\times10^{-3}T + 0.257\times10^{-6}T^{2} + 3.651\times10^{2}T^{-1} - 6.925$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf° = -227.409 + 7.136\times10^{-3}T - 10.833\times10^{-6}T^{2} + 430.600T^{-1}$

$\Delta Gf° = -227.409 - 7.136\times10^{-3}T\ln T + 10.833\times10^{-6}T^{2} + 215.300T^{-1} + 44.319\times10^{-3}T$

453.7-1638 K: $\Delta Hf° = -226.529 - 3.060\times10^{-3}T + 0.095\times10^{-6}T^{2} + 459.200T^{-1}$

$\Delta Gf° = -226.529 + 3.060\times10^{-3}T\ln T - 0.095\times10^{-6}T^{2} + 229.600T^{-1} - 15.104\times10^{-3}T$

1638-2000 K: $\Delta Hf° = -301.462 + 0.112\times10^{-3}T + 0.127\times10^{-6}T^{2} - 636.600T^{-1}$

$\Delta Gf° = -301.462 - 0.112\times10^{-3}T\ln T - 0.127\times10^{-6}T^{2} - 318.300T^{-1} + 54.376\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data from JANAF (60).

$(LiF)_3(g)$

Trimeric Lithium Fluoride (ideal gas)

[Formation: $3Li(c,l,g) + 1.5F_2(g) = (LiF)_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	24.498	75.997	75.997	0	-361.900	-356.674	261.445
300	24.559	76.149	75.999	.045	-361.909	-356.643	259.811
400	27.074	83.592	76.995	2.639	-362.331	-354.819	193.862
453.7	27.858	87.064	77.984	4.120	-362.591	-353.802	170.426
453.7	27.858	87.064	77.984	4.120	-364.742	-353.802	170.426
500	28.534	89.804	78.954	5.425	-365.005	-352.665	154.148
600	29.429	95.092	81.214	8.327	-365.487	-350.149	127.540
700	30.008	99.675	83.531	11.301	-365.885	-347.563	108.513
800	30.402	103.709	85.807	14.322	-366.233	-344.923	94.227
900	30.680	107.307	87.999	17.377	-366.558	-342.238	83.106
1000	30.884	110.551	90.095	20.456	-366.869	-339.520	74.201
1100	31.037	113.502	92.091	23.552	-367.166	-336.770	66.909
1200	31.155	116.207	93.989	26.662	-367.457	-333.995	60.828
1300	31.247	118.705	95.796	29.782	-367.737	-331.195	55.678
1400	31.321	121.023	97.515	32.911	-368.013	-328.373	51.261
1500	31.381	123.186	99.155	36.046	-368.281	-325.534	47.430
1600	31.430	125.213	100.721	39.187	-368.542	-322.672	44.074
1638	31.446	125.951	101.298	40.382	-368.639	-321.584	42.907
1638	31.446	125.951	101.298	40.382	-474.119	-321.584	42.907
1700	31.471	127.120	102.219	42.332	-473.944	-315.807	40.599
1800	31.506	128.920	103.653	45.481	-473.654	-306.515	37.215
1900	31.535	130.624	105.028	48.633	-473.365	-297.237	34.190
2000	31.560	132.242	106.348	51.788	-473.079	-287.971	31.468

Phase changes: 453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.

1638 K, boiling point of Li to monatomic gas; ΔH° = 35.160 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 30.388 + 0.872\times10^{-3}T - 5.467\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 30.388\times10^{-3}T + 0.436\times10^{-6}T^2 + 5.467\times10^{2}T^{-1} - 10.933$

Formation equations (kcal/mol):

298.15-453.7 K: $\Delta Hf^\circ = -366.359 + 12.529\times10^{-3}T - 16.199\times10^{-6}T^2 + 644.950T^{-1}$

$\Delta Gf^\circ = -366.359 - 12.529\times10^{-3}T\ln T + 16.199\times10^{-6}T^2 + 322.475T^{-1} + 95.412\times10^{-3}T$

453.7-1638 K: $\Delta Hf^\circ = -365.040 - 2.765\times10^{-3}T + 0.193\times10^{-6}T^2 + 687.850T^{-1}$

$\Delta Gf^\circ = -365.040 + 2.765\times10^{-3}T\ln T - 0.193\times10^{-6}T^2 + 343.925T^{-1} + 6.277\times10^{-3}T$

1638-2000 K: $\Delta Hf^\circ = -477.439 + 1.993\times10^{-3}T + 0.241\times10^{-6}T^2 - 955.850T^{-1}$

$\Delta Gf^\circ = -477.439 - 1.993\times10^{-3}T\ln T - 0.241\times10^{-6}T^2 - 477.925T^{-1} + 110.497\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data from JANAF (60).

LiI(c,l)
Lithium Iodide
[Formation: $Li(c,l) + 0.5I_2(c,l,g) = LiI(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.200	20.740	20.740	0	-64.630	-64.602	47.354
300	12.214	20.816	20.740	.023	-64.630	-64.602	47.062
386.8	12.766	23.991	21.124	1.109	-64.683	-64.588	36.493
386.8	12.766	23.991	21.124	1.109	-66.537	-64.588	36.493
400	12.850	24.421	21.226	1.278	-66.582	-64.520	35.252
453.7	13.127	26.058	21.703	1.976	-66.768	-64.233	30.941
453.7	13.127	26.058	21.703	1.976	-67.485	-64.233	30.941
458.4	13.151	26.193	21.749	2.037	-67.502	-64.200	30.608
458.4	13.151	26.193	21.749	2.037	-72.513	-64.200	30.608
500	13.366	27.345	22.167	2.589	-72.448	-63.445	27.731
600	13.909	29.829	23.242	3.952	-72.246	-61.662	22.460
700	14.623	32.023	24.343	5.376	-71.972	-59.920	18.708
742	15.010	32.888	24.802	6.000	-71.828	-59.200	17.437
742	15.100	37.605	24.802	9.500	-68.328	-59.200	17.437
800	15.100	38.742	25.772	10.376	-68.115	-58.495	15.980
900	15.100	40.520	27.313	11.886	-67.747	-57.314	13.918
1000	15.100	42.111	28.715	13.396	-67.380	-56.174	12.277
1100	15.100	43.550	29.999	14.906	-67.011	-55.072	10.942
1200	15.100	44.864	31.184	16.416	-66.644	-54.003	9.835
1300	15.100	46.073	32.284	17.926	-66.274	-52.965	8.904
1400	15.100	47.192	33.309	19.436	-65.905	-51.954	8.110

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
453.7 K, melting point of Li; ΔH° = 0.717 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
742 K, melting point of LiI; ΔH° = 3.500 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-742 K: $Cp^\circ = 10.798 + 5.388\times10^{-3}T - 0.182\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 10.798\times10^{-3}T + 2.694\times10^{-6}T^2 + 0.182\times10^{2}T^{-1} - 3.520$

742-1400 K: $Cp^\circ = 15.100$

$H^\circ - H^\circ_{298} = 15.100\times10^{-3}T - 1.704$

LiI(c,l) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -65.451 + 2.661\times10^{-3}T - 3.510\times10^{-6}T^2 + 101.200T^{-1}$

$\Delta Gf^\circ = -65.451 - 2.661\times10^{-3}T\ln T + 3.510\times10^{-6}T^2 + 50.600T^{-1} + 16.388\times10^{-3}T$

386.8-453.7 K: $\Delta Hf^\circ = -66.178 - 0.541\times10^{-3}T - 2.764\times10^{-6}T^2 + 101.200T^{-1}$

$\Delta Gf^\circ = -66.178 + 0.541\times10^{-3}T\ln T + 2.764\times10^{-6}T^2 + 50.600T^{-1} - 0.520\times10^{-3}T$

453.7-458.4 K: $\Delta Hf^\circ = -65.739 - 5.640\times10^{-3}T + 2.700\times10^{-6}T^2 + 115.500T^{-1}$

$\Delta Gf^\circ = -65.739 + 5.640\times10^{-3}T\ln T - 2.700\times10^{-6}T^2 + 57.750T^{-1} - 30.231\times10^{-3}T$

458.4-742 K: $\Delta Hf^\circ = -73.095 - 0.469\times10^{-3}T + 2.666\times10^{-6}T^2 + 107.850T^{-1}$

$\Delta Gf^\circ = -73.095 + 0.469\times10^{-3}T\ln T - 2.666\times10^{-6}T^2 + 53.925T^{-1} + 17.500\times10^{-3}T$

742-1400 K: $\Delta Hf^\circ = -71.279 + 3.833\times10^{-3}T - 0.028\times10^{-6}T^2 + 89.650T^{-1}$

$\Delta Gf^\circ = -71.279 - 3.833\times10^{-3}T\ln T + 0.028\times10^{-6}T^2 + 44.825T^{-1} + 41.504\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Low-temperature heat capacities and entropy at 298 K from Khriplovich (120). High-temperature data based on the relative enthalpy at 742 K and heat capacities at 692 K and 772 K from Dworkin as quoted by JANAF (60). Enthalpy of fusion from Dworkin (65).

LiI(g)

Lithium Iodide (ideal gas)

[Formation: $Li(c,l,g) + 0.5I_2(c,l,g) = LiI(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.263	55.478	55.478	0	-19.380	-29.709	21.777
300	8.270	55.529	55.479	.015	-19.388	-29.774	21.690
386.8	8.518	57.665	55.738	.745	-19.796	-32.726	18.491
386.8	8.518	57.665	55.738	.745	-21.651	-32.726	18.491
400	8.556	57.951	55.806	.858	-21.752	-33.102	18.086
453.7	8.644	59.036	56.127	1.320	-22.173	-34.601	16.667
453.7	8.644	59.036	56.127	1.320	-22.890	-34.601	16.667
458.4	8.652	59.125	56.157	1.361	-22.929	-34.722	16.554
458.4	8.652	59.125	56.157	1.361	-27.939	-34.722	16.554
500	8.720	59.880	56.436	1.722	-28.065	-35.329	15.442
600	8.824	61.480	57.147	2.600	-28.348	-36.755	13.388
700	8.896	62.845	57.865	3.486	-28.612	-38.135	11.906
800	8.950	64.037	58.563	4.379	-28.861	-39.478	10.785
900	8.993	65.094	59.232	5.276	-29.108	-40.791	9.905
1000	9.029	66.043	59.866	6.177	-29.349	-42.075	9.195
1100	9.060	66.905	60.467	7.082	-29.586	-43.336	8.610
1200	9.087	67.695	61.037	7.989	-29.821	-44.577	8.119
1300	9.113	68.423	61.578	8.899	-30.051	-45.797	7.699
1400	9.136	69.099	62.091	9.811	-30.281	-46.999	7.337
1500	9.159	69.730	62.579	10.726	-30.505	-48.186	7.021
1600	9.180	70.322	63.045	11.643	-30.726	-49.356	6.742
1638	9.188	70.538	63.216	11.992	-30.809	-49.798	6.644
1638	9.188	70.538	63.216	11.992	-65.969	-49.798	6.644
1700	9.201	70.879	63.490	12.562	-65.993	-49.184	6.323
1800	9.221	71.406	63.915	13.483	-66.028	-48.196	5.852
1900	9.240	71.905	64.323	14.406	-66.062	-47.204	5.430
2000	9.260	72.379	64.714	15.331	-66.095	-46.209	5.049

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
453.7 K, melting point of Li; $\Delta H°$ = 0.717 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
1638 K, boiling point of Li to monatomic gas; $\Delta H°$ = 35.160 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.843 + 0.230\times10^{-3}T - 0.577\times10^{5}T^{-2}$

$H°- H°_{298} = 8.843\times10^{-3}T + 0.115\times10^{-6}T^{2} + 0.577\times10^{2}T^{-1} - 2.840$

LiI(g) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -19.521 + 0.706\times10^{-3}T - 6.089\times10^{-6}T^2 + 140.700T^{-1}$

$\Delta Gf^\circ = -19.521 - 0.706\times10^{-3}T\ln T + 6.089\times10^{-6}T^2 + 70.350T^{-1} - 32.759\times10^{-3}T$

386.8-453.7 K: $\Delta Hf^\circ = -20.249 - 2.496\times10^{-3}T - 5.343\times10^{-6}T^2 + 140.700T^{-1}$

$\Delta Gf^\circ = -20.249 + 2.496\times10^{-3}T\ln T + 5.343\times10^{-6}T^2 + 70.350T^{-1} - 49.667\times10^{-3}T$

453.7-458.4 K: $\Delta Hf^\circ = -19.809 - 7.595\times10^{-3}T + 0.121\times10^{-6}T^2 + 155.000T^{-1}$

$\Delta Gf^\circ = -19.809 + 7.595\times10^{-3}T\ln T - 0.121\times10^{-6}T^2 + 77.500T^{-1} - 79.379\times10^{-3}T$

458.4-1638 K: $\Delta Hf^\circ = -27.165 - 2.424\times10^{-3}T + 0.087\times10^{-6}T^2 + 147.350T^{-1}$

$\Delta Gf^\circ = -27.165 + 2.424\times10^{-3}T\ln T - 0.087\times10^{-6}T^2 + 73.675T^{-1} - 31.647\times10^{-3}T$

1638-2000 K: $\Delta Hf^\circ = -64.632 - 0.839\times10^{-3}T + 0.103\times10^{-6}T^2 - 400.550T^{-1}$

$\Delta Gf^\circ = -64.632 + 0.839\times10^{-3}T\ln T - 0.103\times10^{-6}T^2 - 200.275T^{-1} + 3.093\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data from JANAF (60).

$(LiI)_2(g)$

Dimeric Lithium Iodide (ideal gas)

[Formation: $2Li(c,l,g) + I_2(c,l,g) = (LiI)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.175	78.997	78.997	.000	-87.000	-98.130	71.930
300	18.193	79.109	78.997	.034	-87.012	-98.199	71.537
386.8	18.787	83.817	79.571	1.642	-87.681	-101.352	57.265
386.8	18.787	83.817	79.571	1.642	-91.390	-101.352	57.265
400	18.877	84.449	79.721	1.891	-91.569	-101.689	55.559
453.7	19.061	86.842	80.424	2.912	-92.315	-103.002	49.616
453.7	19.061	86.842	80.424	2.912	-93.749	-103.002	49.616
458.4	19.077	87.039	80.491	3.001	-93.818	-103.097	49.153
458.4	19.077	87.039	80.491	3.001	-103.839	-103.097	49.153
500	19.219	88.702	81.106	3.798	-104.016	-103.016	45.027
600	19.412	92.225	82.675	5.730	-104.407	-102.779	37.437
700	19.531	95.227	84.258	7.678	-104.758	-102.480	31.995
800	19.610	97.840	85.796	9.635	-105.086	-102.132	27.901
900	19.664	100.153	87.265	11.599	-105.408	-101.743	24.706
1000	19.703	102.227	88.659	13.568	-105.724	-101.318	22.143
1100	19.732	104.106	89.980	15.539	-106.036	-100.863	20.039
1200	19.754	105.824	91.229	17.514	-106.346	-100.380	18.281
1300	19.771	107.406	92.414	19.490	-106.651	-99.870	16.789
1400	19.785	108.872	93.538	21.468	-106.955	-99.336	15.507
1500	19.796	110.237	94.606	23.447	-107.255	-98.783	14.392
1600	19.805	111.515	95.623	25.427	-107.551	-98.205	13.414
1638	19.808	111.980	95.997	26.180	-107.662	-97.984	13.073
1638	19.808	111.980	95.997	26.180	-177.982	-97.984	13.073
1700	19.813	112.716	96.594	27.408	-177.942	-94.953	12.207
1800	19.819	113.849	97.521	29.390	-177.871	-90.074	10.936
1900	19.825	114.920	98.408	31.372	-177.804	-85.198	9.800
2000	19.829	115.937	99.260	33.354	-177.738	-80.324	8.777

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
453.7 K, melting point of Li; $\Delta H°$ = 0.717 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
1638 K, boiling point of Li to monatomic gas; $\Delta H°$ = 35.160 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.766 + 0.068\times10^{-3}T - 1.432\times10^{5}T^{-2}$

$H°- H°_{298} = 19.766\times10^{-3}T + 0.034\times10^{-6}T^{2} + 1.432\times10^{2}T^{-1} - 6.377$

$(LiI)_2(g)$ - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -87.978 + 3.491\times10^{-3}T - 12.374\times10^{-6}T^2 + 309.200T^{-1}$

$\Delta Gf^\circ = -87.978 - 3.491\times10^{-3}T\ln T + 12.374\times10^{-6}T^2 + 154.600T^{-1} - 19.589\times10^{-3}T$

386.8-453.7 K: $\Delta Hf^\circ = -89.433 - 2.913\times10^{-3}T - 10.882\times10^{-6}T^2 + 309.200T^{-1}$

$\Delta Gf^\circ = -89.433 + 2.913\times10^{-3}T\ln T + 10.882\times10^{-6}T^2 + 154.600T^{-1} - 53.404\times10^{-3}T$

453.7-458.4 K: $\Delta Hf^\circ = -88.554 - 13.109\times10^{-3}T + 0.046\times10^{-6}T^2 + 337.800T^{-1}$

$\Delta Gf^\circ = -88.554 + 13.109\times10^{-3}T\ln T - 0.046\times10^{-6}T^2 + 168.900T^{-1} - 112.828\times10^{-3}T$

458.4-1638 K: $\Delta Hf^\circ = -103.267 - 2.769\times10^{-3}T - 0.022\times10^{-6}T^2 + 322.500T^{-1}$

$\Delta Gf^\circ = -103.267 + 2.769\times10^{-3}T\ln T + 0.022\times10^{-6}T^2 + 161.250T^{-1} - 17.365\times10^{-3}T$

1638-2000 K: $\Delta Hf^\circ = -178.199 + 0.403\times10^{-3}T + 0.010\times10^{-6}T^2 - 773.300T^{-1}$

$\Delta Gf^\circ = -178.199 - 0.403\times10^{-3}T\ln T - 0.010\times10^{-6}T^2 - 386.650T^{-1} + 52.115\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data from JANAF (60).

$LuCl_3(g)$

Lutetium Trichloride (ideal gas)

[Formation: $Lu(c,l) + 1.5Cl_2(g) = LuCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.656	84.218	84.218	0	-149.700	-147.346	108.006
300	18.669	84.333	84.218	.035	-149.699	-147.330	107.329
400	19.161	89.780	84.957	1.929	-149.691	-146.544	80.067
500	19.406	94.085	86.367	3.859	-149.685	-145.756	63.709
600	19.544	97.636	87.958	5.807	-149.688	-144.970	52.805
700	19.629	100.656	89.562	7.766	-149.700	-144.182	45.015
800	19.685	103.281	91.116	9.732	-149.734	-143.389	39.171
900	19.724	105.602	92.600	11.702	-149.788	-142.593	34.626
1000	19.752	107.681	94.005	13.676	-149.867	-141.790	30.988
1100	19.772	109.565	95.336	15.652	-149.974	-140.982	28.010
1200	19.788	111.286	96.594	17.630	-150.114	-140.156	25.526
1300	19.800	112.870	97.785	19.610	-150.291	-139.323	23.422
1400	19.810	114.338	98.917	21.590	-150.509	-138.463	21.615
1500	19.818	115.705	99.990	23.572	-150.771	-137.594	20.047
1600	19.825	116.984	101.013	25.554	-151.084	-136.709	18.673
1700	19.830	118.186	101.988	27.537	-151.447	-135.807	17.459
1800	19.835	119.320	102.920	29.520	-151.871	-134.867	16.375
1900	19.838	120.392	103.811	31.503	-152.354	-133.914	15.403
1936	19.839	120.764	104.123	32.217	-152.541	-133.570	15.078
1936	19.839	120.764	104.123	32.217	-156.998	-133.570	15.078
2000	19.842	121.410	104.667	33.487	-157.337	-132.774	14.509

Phase change: 1936 K, melting point of Lu; $\Delta H° = 4.457$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.799 + 0.046\times10^{-3}T - 1.028\times10^{5}T^{-2}$

$H°- H°_{298} = 19.799\times10^{-3}T + 0.023\times10^{-6}T^2 + 1.028\times10^{2}T^{-1} - 6.250$

Formation equations (kcal/mol):

298.15-1936 K: $\Delta Hf° = -150.763 + 2.662\times10^{-3}T - 1.863\times10^{-6}T^2 + 129.850T^{-1}$

$\Delta Gf° = -150.763 - 2.662\times10^{-3}T\ln T + 1.863\times10^{-6}T^2 + 64.925T^{-1} + 25.342\times10^{-3}T$

1936-2000 K: $\Delta Hf° = -147.105 - 4.891\times10^{-3}T - 0.109\times10^{-6}T^2 + 0.350T^{-1}$

$\Delta Gf° = -147.105 + 4.891\times10^{-3}T\ln T + 0.109\times10^{-6}T^2 + 0.175T^{-1} - 30.298\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166) and Schumm (207). Other data based on Myers (165) and Dieke (56).

LuF_3(c,l)
Lutetium Trifluoride
[Formation: Lu(c) + 1.5F_2(g) = LuF_3(c,l)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	20.810	22.665	22.665	0	-401.800	-383.261	280.934
300	20.845	22.794	22.665	.039	-401.794	-383.146	279.118
400	22.182	28.993	23.500	2.197	-401.431	-376.984	205.972
500	22.977	34.034	25.120	4.457	-401.020	-370.918	162.126
600	23.579	38.278	26.968	6.786	-400.584	-364.939	132.927
700	24.111	41.953	28.852	9.171	-400.125	-359.032	112.093
800	24.626	45.207	30.697	11.608	-399.651	-353.191	96.486
900	25.148	48.137	32.475	14.096	-399.159	-347.412	84.362
1000	25.691	50.815	34.177	16.638	-398.649	-341.691	74.676
1100	26.261	53.290	35.804	19.235	-398.119	-336.024	66.761
1200	26.864	55.600	37.357	21.891	-397.568	-330.401	60.173
1230	27.052	56.266	37.811	22.700	-397.398	-328.724	58.408
1230	25.440	61.132	37.811	28.685	-391.413	-328.724	58.408
1300	25.440	62.540	39.105	30.466	-391.139	-325.167	54.665
1400	25.440	64.425	40.846	33.010	-390.787	-320.098	49.969
1457	25.440	65.441	41.790	34.460	-390.607	-317.226	47.583
1457	24.738	70.403	41.790	41.690	-383.377	-317.226	47.583
1500	26.217	71.144	42.620	42.786	-383.250	-315.274	45.935
1600	29.260	72.936	44.458	45.564	-382.764	-310.760	42.447
1700	31.744	74.787	46.188	48.619	-382.055	-306.288	39.375
1800	33.671	76.659	47.828	51.895	-381.186	-301.846	36.649

Phase changes: 1230 K, α - β transition point of LuF_3; $\Delta H°$ = 5.985 kcal/mol.
1457 K, melting point of LuF_3; $\Delta H°$ = 7.230 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1230 K: $Cp° = 21.305 + 4.590\times10^{-3}T - 1.657\times10^{5}T^{-2}$
$H°- H°_{298} = 21.305\times10^{-3}T + 2.295\times10^{-6}T^{2} + 1.657\times10^{2}T^{-1} - 7.112$

1230-1457 K: $Cp° = 25.440$
$H°- H°_{298} = 25.440\times10^{-3}T - 2.606$

1457-1800 K: $Cp° = 51.352 - 0.128\times10^{-3}T - 561.030\times10^{5}T^{-2}$
$H°- H°_{298} = 51.352\times10^{-3}T - 0.064\times10^{-6}T^{2} + 561.030\times10^{2}T^{-1} - 71.500$

Formation equations (kcal/mol):

298.15-1230 K: $\Delta Hf° = -403.695 + 4.646\times10^{-3}T + 0.280\times10^{-6}T^{2} + 144.450T^{-1}$
$\Delta Gf° = -403.695 - 4.646\times10^{-3}T\ln T - 0.280\times10^{-6}T^{2} + 72.225T^{-1} + 94.276\times10^{-3}T$

1230-1457 K: $\Delta Hf° = -399.189 + 8.781\times10^{-3}T - 2.015\times10^{-6}T^{2} - 21.250T^{-1}$
$\Delta Gf° = -399.189 - 8.781\times10^{-3}T\ln T + 2.015\times10^{-6}T^{2} - 10.625T^{-1} + 117.264\times10^{-3}T$

1457-1800 K: $\Delta Hf° = -468.083 + 34.693\times10^{-3}T - 2.079\times10^{-6}T^{2} + 56081.750T^{-1}$
$\Delta Gf° = -468.083 - 34.693\times10^{-3}T\ln T + 2.079\times10^{-6}T^{2} + 28040.875T^{-1} + 339.988\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K and low-temperature heat capacities from Flotow (81). High-temperature data based on Spedding (223).

$LuF_3(g)$

Lutetium Trifluoride (ideal gas)

[Formation: $Lu(c,l) + 1.5F_2(g) = LuF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	16.869	75.354	75.354	0	-297.900	-295.070	216.290
300	16.894	75.458	75.355	.031	-297.902	-295.053	214.943
400	17.949	80.477	76.032	1.778	-297.949	-294.096	160.685
500	18.553	84.553	77.341	3.606	-297.971	-293.128	128.125
600	18.920	87.971	78.836	5.481	-297.990	-292.160	106.418
700	19.156	90.907	80.356	7.386	-298.010	-291.185	90.911
800	19.315	93.476	81.839	9.310	-298.049	-290.204	79.279
900	19.427	95.757	83.260	11.247	-298.108	-289.219	70.231
1000	19.509	97.809	84.615	13.194	-298.193	-288.229	62.992
1100	19.570	99.671	85.900	15.148	-298.306	-287.230	57.067
1200	19.617	101.376	87.119	17.108	-298.451	-286.215	52.126
1300	19.654	102.948	88.278	19.071	-298.634	-285.192	47.945
1400	19.683	104.405	89.378	21.038	-298.859	-284.142	44.356
1500	19.707	105.764	90.425	23.008	-299.129	-283.082	41.245
1600	19.727	107.037	91.424	24.980	-299.448	-282.005	38.520
1700	19.743	108.233	92.378	26.953	-299.820	-280.912	36.113
1800	19.757	109.362	93.291	28.928	-300.253	-279.778	33.969
1900	19.769	110.430	94.165	30.904	-300.745	-278.633	32.050
1936	19.773	110.801	94.471	31.616	-300.936	-278.219	31.407
1936	19.773	110.801	94.471	31.616	-305.393	-278.219	31.407
2000	19.779	111.445	95.004	32.882	-305.737	-277.301	30.302

Phase change: 1936 K, melting point of Lu; $\Delta H° = 4.457$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.397 + 0.278\times10^{-3}T - 2.321\times10^{5}T^{-2}$

$H°- H°_{298} = 19.397\times10^{-3}T + 0.139\times10^{-6}T^2 + 2.321\times10^{2}T^{-1} - 6.574$

Formation equations (kcal/mol):

298.15-1936 K: $\Delta Hf° = -299.257 + 2.738\times10^{-3}T - 1.876\times10^{-6}T^2 + 210.850T^{-1}$

$\Delta Gf° = -299.257 - 2.738\times10^{-3}T\ln T + 1.876\times10^{-6}T^2 + 105.425T^{-1} + 27.896\times10^{-3}T$

1936-2000 K: $\Delta Hf° = -295.598 - 4.815\times10^{-3}T - 0.122\times10^{-6}T^2 + 81.350T^{-1}$

$\Delta Gf° = -295.598 + 4.815\times10^{-3}T\ln T + 0.122\times10^{-6}T^2 + 40.675T^{-1} - 27.745\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

MgBr(g)

Magnesium Monobromide (ideal gas)

[Formation: $Mg(c,l,g) + 0.5Br_2(l,g) = MgBr(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.518	58.516	58.516	0	-8.400	-18.095	13.264
300	8.523	58.569	58.516	.016	-8.411	-18.154	13.225
332.6	8.586	59.451	58.565	.295	-8.622	-19.201	12.617
332.6	8.586	59.451	58.565	.295	-12.155	-19.201	12.617
400	8.716	61.051	58.854	.879	-12.279	-20.620	11.266
500	8.820	63.008	59.496	1.756	-12.483	-22.685	9.916
600	8.885	64.622	60.219	2.642	-12.707	-24.701	8.997
700	8.929	65.995	60.949	3.532	-12.957	-26.680	8.330
800	8.962	67.190	61.656	4.427	-13.231	-28.625	7.820
900	8.989	68.247	62.330	5.325	-13.534	-30.526	7.413
922	8.994	68.464	62.474	5.523	-13.603	-30.945	7.335
922	8.994	68.464	62.474	5.523	-15.742	-30.945	7.335
1000	9.011	69.195	62.970	6.225	-16.001	-32.225	7.043
1100	9.031	70.055	63.576	7.127	-16.350	-33.833	6.722
1200	9.049	70.841	64.149	8.031	-16.728	-35.408	6.449
1300	9.065	71.566	64.692	8.936	-17.125	-36.937	6.210
1363	9.074	71.996	65.020	9.508	-17.388	-37.910	6.079
1363	9.074	71.996	65.020	9.508	-47.638	-37.910	6.079
1400	9.080	72.239	65.208	9.844	-47.654	-37.647	5.877
1500	9.095	72.866	65.698	10.752	-47.697	-36.933	5.381
1600	9.109	73.453	66.164	11.663	-47.737	-36.212	4.946
1700	9.123	74.006	66.610	12.574	-47.778	-35.493	4.563
1800	9.136	74.527	67.034	13.487	-47.817	-34.766	4.221
1900	9.149	75.022	67.443	14.401	-47.856	-34.040	3.915
2000	9.162	75.491	67.832	15.317	-47.894	-33.311	3.640

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.
922 K, melting point of Mg; $\Delta H° = 2.139$ kcal/mol.
1363 K, boiling point of Mg; $\Delta H° = 30.250$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.909 + 0.136\times10^{-3}T - 0.384\times10^{5}T^{-2}$

$H°- H°_{298} = 8.909\times10^{-3}T + 0.068\times10^{-6}T^{2} + 0.384\times10^{2}T^{-1} - 2.791$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -6.835 - 5.280\times10^{-3}T - 1.270\times10^{-6}T^{2} + 36.500T^{-1}$

$\Delta Gf° = -6.835 + 5.280\times10^{-3}T\ln T + 1.270\times10^{-6}T^{2} + 18.250T^{-1} - 68.428\times10^{-3}T$

332.6-922 K: $\Delta Hf° = -11.836 - 0.699\times10^{-3}T - 1.348\times10^{-6}T^{2} + 20.800T^{-1}$

$\Delta Gf° = -11.836 + 0.699\times10^{-3}T\ln T + 1.348\times10^{-6}T^{2} + 10.400T^{-1} - 26.751\times10^{-3}T$

922-1363 K: $\Delta Hf° = -13.159 - 1.565\times10^{-3}T - 1.034\times10^{-6}T^{2} - 240.900T^{-1}$

$\Delta Gf° = -13.159 + 1.565\times10^{-3}T\ln T + 1.034\times10^{-6}T^{2} - 120.450T^{-1} - 30.784\times10^{-3}T$

1363-2000 K: $\Delta Hf° = -47.017 - 0.524\times10^{-3}T + 0.040\times10^{-6}T^{2} + 22.700T^{-1}$

$\Delta Gf° = -47.017 + 0.524\times10^{-3}T\ln T - 0.040\times10^{-6}T^{2} + 11.350T^{-1} + 2.963\times10^{-3}T$

Source: Data from Chase (26).

$MgBr_2(c,l)$
Magnesium Dibromide
[Formation: $Mg(c,l,g) + Br_2(l,g) = MgBr_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	17.846	28.000	28.000	0	-125.300	-120.473	88.308
300	17.540	28.109	28.001	.032	-125.312	-120.442	87.741
332.6	17.843	29.933	28.103	.609	-125.519	-119.902	78.786
332.6	17.843	29.933	28.103	.609	-132.584	-119.902	78.786
400	18.470	33.290	28.700	1.836	-132.360	-117.357	64.120
500	19.059	37.478	30.050	3.714	-132.003	-113.650	49.676
600	19.462	40.989	31.589	5.640	-131.631	-110.010	40.071
700	19.830	44.017	33.153	7.605	-131.253	-106.436	33.230
800	20.209	46.689	34.681	9.606	-130.869	-102.919	28.116
900	20.619	49.093	36.152	11.647	-130.478	-99.445	24.148
922	20.717	49.592	36.467	12.102	-130.389	-98.692	23.393
922	20.717	49.592	36.467	12.102	-132.528	-98.692	23.393
984	20.994	50.949	37.336	13.395	-132.277	-96.429	21.417
984	25.000	60.502	37.336	22.795	-122.877	-96.429	21.417
1000	25.000	60.905	37.710	23.195	-122.747	-96.000	20.981
1100	25.000	63.287	39.928	25.695	-121.949	-93.366	18.550
1200	25.000	65.463	41.967	28.195	-121.182	-90.804	16.537
1300	25.000	67.464	43.852	30.695	-120.437	-88.291	14.843
1363	25.000	68.647	44.972	32.270	-119.983	-86.763	13.912
1363	25.000	68.647	44.972	32.270	-150.233	-86.763	13.912
1400	25.000	69.317	45.606	33.195	-149.827	-85.046	13.276
1431	25.000	69.865	46.126	33.970	-149.487	-83.616	12.770

*Data estimated except enthalpy of formation at 298 K and temperature of fusion.

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
922 K, melting point of Mg; $\Delta H°$ = 2.139 kcal/mol.
984 K, melting point of $MgBr_2$; $\Delta H°$ = 9.400 kcal/mol.
1363 K, boiling point of Mg; $\Delta H°$ = 30.250 kcal/mol.
1431 K, boiling point of $MgBr_2$ to monomer; $\Delta H°$ = 35.6 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-984 K: $Cp° = 16.851 + 4.318\times10^{-3}T - 0.260\times10^{5}T^{-2}$

$H°- H°_{298} = 16.851\times10^{-3}T + 2.159\times10^{-6}T^{2} + 0.260\times10^{2}T^{-1} - 5.303$

984-1431 K: $Cp° = 25.000$

$H°- H°_{298} = 25.000\times10^{-3}T - 1.805$

$MgBr_2$(c,l) - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -123.555 - 6.383\times10^{-3}T + 0.871\times10^{-6}T^2 + 24.100T^{-1}$

$\Delta Gf^\circ = -123.555 + 6.383\times10^{-3}T\ln T - 0.871\times10^{-6}T^2 + 12.050T^{-1} - 25.907\times10^{-3}T$

332.6-922 K: $\Delta Hf^\circ = -133.556 + 2.778\times10^{-3}T + 0.716\times10^{-6}T^2 - 7.300T^{-1}$

$\Delta Gf^\circ = -133.556 - 2.778\times10^{-3}T\ln T - 0.716\times10^{-6}T^2 - 3.650T^{-1} + 57.448\times10^{-3}T$

922-984 K: $\Delta Hf^\circ = -134.879 + 1.912\times10^{-3}T + 1.030\times10^{-6}T^2 - 269.000T^{-1}$

$\Delta Gf^\circ = -134.879 - 1.912\times10^{-3}T\ln T - 1.030\times10^{-6}T^2 - 134.500T^{-1} + 53.416\times10^{-3}T$

984-1363 K: $\Delta Hf^\circ = -131.381 + 10.061\times10^{-3}T - 1.129\times10^{-6}T^2 - 295.000T^{-1}$

$\Delta Gf^\circ = -131.381 - 10.061\times10^{-3}T\ln T + 1.129\times10^{-6}T^2 - 147.500T^{-1} + 103.909\times10^{-3}T$

1363-1431 K: $\Delta Hf^\circ = -165.238 + 11.102\times10^{-3}T - 0.055\times10^{-6}T^2 - 31.400T^{-1}$

$\Delta Gf^\circ = -165.238 - 11.102\times10^{-3}T\ln T + 0.055\times10^{-6}T^2 - 15.700T^{-1} + 137.656\times10^{-3}T$

Source: Data from Chase (27) who estimated all except enthalpy of formation at 298 K and temperature of fusion.

$MgBr_2(g)$

Magnesium Dibromide (ideal gas)

[Formation: $Mg(c,l,g) + Br_2(l,g) = MgBr_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	14.032	71.922	71.922	0	-72.400	-80.669	59.131
300	14.041	72.009	71.922	.026	-72.418	-80.718	58.803
332.6	14.149	73.463	72.003	.485	-72.742	-81.604	53.621
332.6	14.149	73.463	72.003	.485	-79.807	-81.604	53.621
400	14.372	76.099	72.479	1.448	-79.848	-81.969	44.785
500	14.548	79.327	73.537	2.895	-79.922	-82.494	36.057
600	14.651	81.989	74.729	4.356	-80.015	-82.994	30.230
700	14.715	84.253	75.933	5.824	-80.134	-83.482	26.064
800	14.758	86.221	77.099	7.298	-80.277	-83.953	22.935
900	14.788	87.961	78.211	8.775	-80.450	-84.398	20.494
922	14.793	88.318	78.448	9.100	-80.490	-84.498	20.029
922	14.793	88.318	78.448	9.100	-82.629	-84.498	20.029
1000	14.809	89.520	79.265	10.255	-82.787	-84.655	18.501
1100	14.825	90.932	80.262	11.737	-83.007	-84.833	16.855
1200	14.838	92.223	81.206	13.220	-83.257	-84.991	15.479
1300	14.847	93.411	82.100	14.704	-83.528	-85.113	14.309
1363	14.852	94.114	82.640	15.639	-83.713	-85.205	13.662
1363	14.852	94.114	82.640	15.639	-113.963	-85.205	13.662
1400	14.855	94.512	82.948	16.189	-113.933	-84.425	13.179
1500	14.861	95.537	83.754	17.675	-113.852	-82.322	11.994
1600	14.866	96.496	84.520	19.162	-113.771	-80.221	10.957
1700	14.871	97.397	85.251	20.649	-113.691	-78.127	10.044
1800	14.874	98.247	85.949	22.136	-113.611	-76.036	9.232
1900	14.877	99.052	86.619	23.623	-113.533	-73.950	8.506
2000	14.880	99.815	87.260	25.111	-113.456	-71.870	7.853

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
922 K, melting point of Mg; $\Delta H°$ = 2.139 kcal/mol.
1363 K, boiling point of Mg; $\Delta H°$ = 30.250 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 14.805 + 0.062\times10^{-3}T - 0.704\times10^{5}T^{-2}$

$H°- H°_{298} = 14.805\times10^{-3}T + 0.031\times10^{-6}T^2 + 0.704\times10^{2}T^{-1} - 4.653$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -70.005 - 8.429\times10^{-3}T - 1.257\times10^{-6}T^2 + 68.500T^{-1}$

$\Delta Gf° = -70.005 + 8.429\times10^{-3}T\ln T + 1.257\times10^{-6}T^2 + 34.250T^{-1} - 84.551\times10^{-3}T$

332.6-922 K: $\Delta Hf° = -80.005 + 0.732\times10^{-3}T - 1.412\times10^{-6}T^2 + 37.100T^{-1}$

$\Delta Gf° = -80.005 - 0.732\times10^{-3}T\ln T + 1.412\times10^{-6}T^2 + 18.550T^{-1} - 1.196\times10^{-3}T$

922-1363 K: $\Delta Hf° = -81.329 - 0.134\times10^{-3}T - 1.098\times10^{-6}T^2 - 224.600T^{-1}$

$\Delta Gf° = -81.329 + 0.134\times10^{-3}T\ln T + 1.098\times10^{-6}T^2 - 112.300T^{-1} - 5.229\times10^{-3}T$

1363-2000 K: $\Delta Hf° = -115.186 + 0.907\times10^{-3}T - 0.024\times10^{-6}T^2 + 39.000T^{-1}$

$\Delta Gf° = -115.186 - 0.907\times10^{-3}T\ln T + 0.024\times10^{-6}T^2 + 19.500T^{-1} + 28.518\times10^{-3}T$

Source: Data from Chase (27) who estimated some molecular constants.

$(MgBr_2)_2(g)$

Dimeric Magnesium Dibromide (ideal gas)

[Formation: $2Mg(c,l,g) + 2Br_2(l,g) = (MgBr_2)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	30.834	110.237	110.237	0	-183.500	-190.017	139.285
300	30.846	110.428	110.238	.057	-183.531	-190.055	138.453
332.6	30.979	113.617	110.416	1.065	-184.091	-190.735	125.330
332.6	30.979	113.617	110.416	1.065	-198.221	-190.735	125.330
400	31.253	119.365	111.452	3.165	-198.127	-189.235	103.392
500	31.445	126.362	113.760	6.301	-198.033	-187.030	81.750
600	31.551	132.105	116.353	9.451	-197.991	-184.825	67.322
700	31.615	136.974	118.960	12.610	-198.006	-182.630	57.019
800	31.657	141.199	121.483	15.773	-198.077	-180.435	49.292
900	31.686	144.929	123.883	18.941	-198.209	-178.212	43.275
922	31.690	145.694	124.395	19.638	-198.244	-177.731	42.129
922	31.690	145.694	124.395	19.638	-202.522	-177.731	42.129
1000	31.706	148.269	126.159	22.110	-202.674	-175.639	38.385
1100	31.722	151.291	128.307	25.282	-202.906	-172.928	34.357
1200	31.733	154.052	130.340	28.454	-203.200	-170.195	30.996
1300	31.742	156.592	132.263	31.628	-203.536	-167.406	28.143
1363	31.747	158.095	133.422	33.628	-203.777	-165.687	26.567
1363	31.747	158.095	133.422	33.628	-264.277	-165.687	26.567
1400	31.750	158.945	134.086	34.803	-264.141	-163.015	25.447
1500	31.755	161.136	135.817	37.978	-263.776	-155.809	22.701
1600	31.760	163.185	137.464	41.154	-263.412	-148.620	20.300
1700	31.764	165.111	139.035	44.330	-263.050	-141.461	18.186
1800	31.767	166.927	140.534	47.507	-262.687	-134.316	16.308
1900	31.770	168.644	141.968	50.684	-262.328	-127.189	14.630
2000	31.773	170.274	143.344	53.861	-261.973	-120.089	13.123

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.
922 K, melting point of Mg; $\Delta H° = 2.139$ kcal/mol.
1363 K, boiling point of Mg; $\Delta H° = 30.250$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 31.781 + 0.008\times10^{-3}T - 0.844\times10^{5}T^{-2}$

$H°- H°_{298} = 31.781\times10^{-3}T + 0.004\times10^{-6}T^2 + 0.844\times10^{2}T^{-1} - 9.759$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -179.163 - 14.687\times10^{-3}T - 2.572\times10^{-6}T^2 + 80.600T^{-1}$

$\Delta Gf° = -179.163 + 14.687\times10^{-3}T\ln T + 2.572\times10^{-6}T^2 + 40.300T^{-1} - 121.307\times10^{-3}T$

332.6-922 K: $\Delta Hf° = -199.164 + 3.635\times10^{-3}T - 2.882\times10^{-6}T^2 + 17.800T^{-1}$

$\Delta Gf° = -199.164 - 3.635\times10^{-3}T\ln T + 2.882\times10^{-6}T^2 + 8.900T^{-1} + 45.403\times10^{-3}T$

922-1363 K: $\Delta Hf° = -201.811 + 1.903\times10^{-3}T - 2.254\times10^{-6}T^2 - 505.600T^{-1}$

$\Delta Gf° = -201.811 - 1.903\times10^{-3}T\ln T + 2.254\times10^{-6}T^2 - 252.800T^{-1} + 37.338\times10^{-3}T$

1363-2000 K: $\Delta Hf° = -269.526 + 3.985\times10^{-3}T - 0.106\times10^{-6}T^2 + 21.600T^{-1}$

$\Delta Gf° = -269.526 - 3.985\times10^{-3}T\ln T + 0.106\times10^{-6}T^2 + 10.800T^{-1} + 104.831\times10^{-3}T$

Source: Data from Chase (27) who estimated molecular constants.

MgCl(g)

Magnesium Monochloride (ideal gas)

[Formation: $Mg(c,l,g) + 0.5Cl_2(g) = MgCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.324	55.760	55.760	0	-10.400	-16.752	12.279
300	8.330	55.812	55.762	.015	-10.403	-16.791	12.232
400	8.587	58.247	56.090	.863	-10.580	-18.894	10.323
500	8.730	60.180	56.722	1.729	-10.780	-20.953	9.158
600	8.819	61.780	57.435	2.607	-11.002	-22.963	8.364
700	8.878	63.145	58.156	3.492	-11.250	-24.937	7.786
800	8.922	64.333	58.855	4.382	-11.526	-26.877	7.342
900	8.956	65.386	59.524	5.276	-11.828	-28.772	6.987
922	8.962	65.602	59.666	5.473	-11.897	-29.190	6.919
922	8.962	65.602	59.666	5.473	-14.036	-29.190	6.919
1000	8.983	66.331	60.158	6.173	-14.295	-30.467	6.658
1100	9.007	67.188	60.758	7.073	-14.643	-32.069	6.371
1200	9.027	67.973	61.328	7.974	-15.022	-33.640	6.127
1300	9.046	68.696	61.867	8.878	-15.419	-35.162	5.911
1363	9.057	69.124	62.193	9.448	-15.684	-36.133	5.794
1363	9.057	69.124	62.193	9.448	-45.934	-36.133	5.794
1400	9.063	69.367	62.379	9.783	-45.950	-35.867	5.599
1500	9.079	69.993	62.866	10.691	-45.992	-35.146	5.121
1600	9.094	70.580	63.331	11.599	-46.035	-34.423	4.702
1700	9.109	71.131	63.773	12.509	-46.076	-33.695	4.332
1800	9.123	71.652	64.196	13.421	-46.116	-32.964	4.002
1900	9.136	72.146	64.602	14.334	-46.156	-32.232	3.707
2000	9.150	72.615	64.991	15.248	-46.197	-31.498	3.442

Phase changes: 922 K, melting point of Mg; $\Delta H°$ = 2.139 kcal/mol.
1363 K, boiling point of Mg; $\Delta H°$ = 30.250 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.865 + 0.162\times10^{-3}T - 0.524\times10^{5}T^{-2}$

$H°- H°_{298} = 8.865\times10^{-3}T + 0.081\times10^{-6}T^{2} + 0.524\times10^{2}T^{-1} - 2.826$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf° = -10.129 - 0.692\times10^{-3}T - 1.351\times10^{-6}T^{2} + 16.350T^{-1}$

$\Delta Gf° = -10.129 + 0.692\times10^{-3}T\ln T + 1.351\times10^{-6}T^{2} + 8.175T^{-1} - 26.650\times10^{-3}T$

922-1363 K: $\Delta Hf° = -11.452 - 1.558\times10^{-3}T - 1.037\times10^{-6}T^{2} - 245.350T^{-1}$

$\Delta Gf° = -11.452 + 1.558\times10^{-3}T\ln T + 1.037\times10^{-6}T^{2} - 122.675T^{-1} - 30.683\times10^{-3}T$

1363-2000 K: $\Delta Hf° = -45.310 - 0.517\times10^{-3}T + 0.037\times10^{-6}T^{2} + 18.250T^{-1}$

$\Delta Gf° = -45.310 + 0.517\times10^{-3}T\ln T - 0.037\times10^{-6}T^{2} + 9.125T^{-1} + 3.064\times10^{-3}T$

Source: Data from JANAF (60).

$MgCl_2(c,l)$
Magnesium Dichloride
[Formation: $Mg(c,l,g) + Cl_2(g) = MgCl_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	17.040	21.400	21.400	0	-153.990	-142.153	104.200
300	17.076	21.506	21.400	.032	-153.984	-142.079	103.503
400	18.239	26.606	22.089	1.807	-153.649	-138.161	75.487
500	18.714	30.733	23.417	3.658	-153.290	-134.332	58.716
600	19.011	34.172	24.932	5.544	-152.939	-130.570	47.560
700	19.304	37.124	26.467	7.460	-152.595	-126.869	39.610
800	19.667	39.724	27.964	9.408	-152.255	-123.220	33.662
900	20.133	42.067	29.404	11.397	-151.907	-119.606	29.044
922	20.260	42.555	29.712	11.841	-151.827	-118.821	28.165
922	20.260	42.555	29.712	11.841	-153.966	-118.821	28.165
980	20.594	43.800	30.509	13.025	-153.754	-116.623	26.008
980	22.180	53.540	30.509	22.570	-144.209	-116.623	26.008
1000	22.180	53.988	30.974	23.014	-144.101	-116.061	25.365
1100	22.180	56.102	33.164	25.232	-143.580	-113.285	22.507
1200	22.180	58.032	35.157	27.450	-143.092	-110.555	20.135
1300	22.180	59.807	36.985	29.668	-142.626	-107.850	18.131
1363	22.180	60.857	38.065	31.065	-142.348	-106.191	17.027
1363	22.180	60.857	38.065	31.065	-172.598	-106.191	17.027
1400	22.180	61.451	38.675	31.886	-172.296	-104.393	16.296
1500	22.180	62.981	40.245	34.104	-171.481	-99.573	14.508

Phase changes: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
980 K, melting point of $MgCl_2$; ΔH° = 9.545 kcal/mo.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-980 K: $Cp^\circ = 18.262 + 2.212\times10^{-3}T - 1.671\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 18.262\times10^{-3}T + 1.106\times10^{-6}T^2 + 1.671\times10^{2}T^{-1} - 6.104$

980-1500 K: $Cp^\circ = 22.180$
$H^\circ - H^\circ_{298} = 22.180\times10^{-3}T + 0.834$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf^\circ = -155.562 + 4.292\times10^{-3}T - 0.370\times10^{-6}T^2 + 96.900T^{-1}$
$\Delta Gf^\circ = -155.562 - 4.292\times10^{-3}T\ln T + 0.370\times10^{-6}T^2 + 48.450T^{-1} + 68.770\times10^{-3}T$

922-980 K: $\Delta Hf^\circ = -156.885 + 3.426\times10^{-3}T - 0.056\times10^{-6}T^2 - 164.800T^{-1}$
$\Delta Gf^\circ = -156.885 - 3.426\times10^{-3}T\ln T + 0.056\times10^{-6}T^2 - 82.400T^{-1} + 64.738\times10^{-3}T$

980-1363 K: $\Delta Hf^\circ = -149.947 + 7.344\times10^{-3}T - 1.162\times10^{-6}T^2 - 331.900T^{-1}$
$\Delta Gf^\circ = -149.947 - 7.344\times10^{-3}T\ln T + 1.162\times10^{-6}T^2 - 165.950T^{-1} + 83.647\times10^{-3}T$

1363-1500 K: $\Delta Hf^\circ = -183.805 + 8.385\times10^{-3}T - 0.088\times10^{-6}T^2 - 68.300T^{-1}$
$\Delta Gf^\circ = -183.805 - 8.385\times10^{-3}T\ln T + 0.088\times10^{-6}T^2 - 34.150T^{-1} + 117.393\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Shin (211). Low-temperature heat capacities and entropy at 298 K from Kelley (119). High-temperature data for crystal based on Moore (160). Temperature and enthalpy of fusion and heat capacity of liquid based on Holm (101).

$MgCl_2(g)$

Magnesium Dichloride (ideal gas)

[Formation: $Mg(c,l,g) + Cl_2(g) = MgCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	13.646	66.184	66.184	0	-93.800	-95.316	69.867
300	13.658	66.268	66.185	.025	-93.801	-95.324	69.443
400	14.115	70.267	66.727	1.416	-93.850	-95.827	52.357
500	14.368	73.446	67.762	2.842	-93.916	-96.314	42.098
600	14.519	76.080	68.937	4.286	-94.007	-96.783	35.253
700	14.615	78.326	70.122	5.743	-94.122	-97.237	30.358
800	14.680	80.282	71.272	7.208	-94.265	-97.676	26.684
900	14.725	82.014	72.371	8.679	-94.435	-98.086	23.818
922	14.732	82.370	72.605	9.003	-94.475	-98.179	23.272
922	14.732	82.370	72.605	9.003	-96.614	-98.179	23.272
1000	14.758	83.567	73.414	10.153	-96.772	-98.311	21.486
1100	14.783	84.975	74.402	11.630	-96.992	-98.457	19.561
1200	14.802	86.262	75.338	13.109	-97.243	-98.582	17.954
1300	14.816	87.447	76.224	14.590	-97.514	-98.670	16.588
1363	14.824	88.149	76.759	15.524	-97.699	-98.741	15.832
1363	14.824	88.149	76.759	15.524	-127.949	-98.741	15.832
1400	14.828	88.546	77.065	16.073	-127.919	-97.949	15.290
1500	14.838	89.569	77.865	17.556	-127.839	-95.813	13.960
1600	14.846	90.527	78.627	19.040	-127.760	-93.680	12.796
1700	14.852	91.427	79.353	20.525	-127.681	-91.551	11.770
1800	14.858	92.276	80.048	22.010	-127.603	-89.429	10.858
1900	14.862	93.080	80.714	23.496	-127.526	-87.309	10.043
2000	14.866	93.842	81.351	24.983	-127.451	-85.193	9.309

Phase changes: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 14.719 + 0.114\times10^{-3}T - 0.984\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.719\times10^{-3}T + 0.057\times10^{-5}T^2 + 0.984\times10^{2}T^{-1} - 4.724$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf^\circ = -93.992 + 0.749\times10^{-3}T - 1.419\times10^{-6}T^2 + 28.200T^{-1}$

$\Delta Gf^\circ = -93.992 - 0.749\times10^{-3}T\ln T + 1.419\times10^{-6}T^2 + 14.100T^{-1} - 0.755\times10^{-3}T$

922-1363 K: $\Delta Hf^\circ = -95.315 - 0.117\times10^{-3}T - 1.105\times10^{-6}T^2 - 233.500T^{-1}$

$\Delta Gf^\circ = -95.315 + 0.117\times10^{-3}T\ln T + 1.105\times10^{-6}T^2 - 116.750T^{-1} - 4.788\times10^{-3}T$

1363-2000 K: $\Delta Hf^\circ = -129.173 + 0.924\times10^{-3}T - 0.031\times10^{-6}T^2 + 30.100T^{-1}$

$\Delta Gf^\circ = -129.173 - 0.924\times10^{-3}T\ln T + 0.031\times10^{-6}T^2 + 15.050T^{-1} + 28.959\times10^{-3}T$

Source: Data from JANAF (60).

$(MgCl_2)_2(g)$

Dimeric Magnesium Dichloride (ideal gas)

[Formation: $2Mg(c,l,g) + 2Cl_2(g) = (MgCl_2)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	29.543	100.098	100.098	0	-228.100	-221.510	162.369
300	29.567	100.281	100.098	.055	-228.097	-221.467	161.337
400	30.458	108.924	101.272	3.061	-227.971	-219.281	119.808
500	30.911	115.775	103.511	6.132	-227.884	-217.123	94.903
600	31.170	121.435	106.040	9.237	-227.849	-214.966	78.300
700	31.331	126.253	108.592	12.363	-227.867	-212.818	66.444
800	31.437	130.444	111.066	15.502	-227.944	-210.670	57.552
900	31.511	134.152	113.431	18.649	-228.079	-208.493	50.628
922	31.523	134.913	113.934	19.342	-228.114	-208.022	49.309
922	31.523	134.913	113.934	19.342	-232.392	-208.022	49.309
1000	31.564	137.474	115.671	21.803	-232.547	-205.965	45.013
1100	31.603	140.485	117.792	24.962	-232.782	-203.301	40.392
1200	31.634	143.236	119.800	28.123	-233.081	-200.614	36.536
1300	31.657	145.769	121.701	31.288	-233.420	-197.869	33.264
1363	31.669	147.268	122.849	33.283	-233.663	-196.180	31.456
1363	31.669	147.268	122.849	33.283	-294.163	-196.180	31.456
1400	31.676	148.116	123.505	34.455	-294.029	-193.523	30.210
1500	31.691	150.302	125.220	37.623	-293.667	-186.360	27.152
1600	31.704	152.347	126.851	40.793	-293.307	-179.216	24.479
1700	31.714	154.270	128.409	43.964	-292.948	-172.095	22.124
1800	31.723	156.083	129.896	47.136	-292.590	-164.997	20.033
1900	31.730	157.798	131.320	50.308	-292.236	-157.914	18.164
2000	31.736	159.426	132.685	53.482	-291.886	-150.854	16.484

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 922 K, melting point of Mg; $\Delta H° = 2.139$ kcal/mol.
1363 K, boiling point of Mg; $\Delta H° = 30.250$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 31.618 + 0.112\times10^{-3}T - 1.874\times10^{5}T^{-2}$

$H°-H°_{298} = 31.618\times10^{-3}T + 0.056\times10^{-6}T^2 + 1.874\times10^{2}T^{-1} - 10.060$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf° = -229.097 + 3.678\times10^{-3}T - 2.896\times10^{-6}T^2 + 47.000T^{-1}$

$\Delta Gf° = -229.097 - 3.678\times10^{-3}T\ln T + 2.896\times10^{-6}T^2 + 23.500T^{-1} + 45.273\times10^{-3}T$

922-1363 K: $\Delta Hf° = -231.744 + 1.946\times10^{-3}T - 2.268\times10^{-6}T^2 - 476.400T^{-1}$

$\Delta Gf° = -231.744 - 1.946\times10^{-3}T\ln T + 2.268\times10^{-6}T^2 - 238.200T^{-1} + 37.208\times10^{-3}T$

1363-2000 K: $\Delta Hf° = -299.459 + 4.028\times10^{-3}T - 0.120\times10^{-6}T^2 + 50.800T^{-1}$

$\Delta Gf° = -299.459 - 4.028\times10^{-3}T\ln T + 0.120\times10^{-6}T^2 + 25.400T^{-1} + 104.701\times10^{-3}T$

Source: Data from JANAF (60) who estimated most molecular constants.

MgF(g)

Magnesium Monofluoride (ideal gas)

[Formation: $Mg(c,l,g) + 0.5F_2(g) = MgF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.784	52.814	52.814	0	-56.600	-62.796	46.030
300	7.793	52.862	52.815	.014	-56.604	-62.834	45.774
400	8.173	55.159	53.124	.814	-56.799	-64.882	35.449
500	8.420	57.012	53.724	1.644	-57.009	-66.882	29.234
600	8.583	58.562	54.404	2.495	-57.239	-68.831	25.071
700	8.695	59.894	55.095	3.359	-57.493	-70.743	22.087
800	8.776	61.061	55.770	4.233	-57.772	-72.620	19.839
900	8.837	62.098	56.416	5.114	-58.078	-74.452	18.079
922	8.848	62.312	56.554	5.309	-58.148	-74.856	17.743
922	8.848	62.312	56.554	5.309	-60.287	-74.856	17.743
1000	8.885	63.032	57.032	6.000	-60.549	-76.083	16.628
1100	8.924	63.880	57.615	6.891	-60.901	-77.621	15.422
1200	8.957	64.658	58.170	7.785	-61.283	-79.127	14.411
1300	8.985	65.376	58.698	8.682	-61.683	-80.585	13.547
1363	9.000	65.802	59.016	9.249	-61.950	-81.515	13.070
1363	9.000	65.802	59.016	9.249	-92.200	-81.515	13.070
1400	9.009	66.043	59.199	9.582	-92.217	-81.226	12.680
1500	9.031	66.666	59.677	10.484	-92.263	-80.441	11.720
1600	9.051	67.249	60.132	11.388	-92.310	-79.650	10.880
1700	9.070	67.798	60.566	12.294	-92.354	-78.857	10.138
1800	9.088	68.317	60.983	13.202	-92.398	-78.062	9.478
1900	9.104	68.809	61.382	14.111	-92.443	-77.264	8.887
2000	9.120	69.276	61.765	15.022	-92.488	-76.464	8.355

Phase changes: 922 K, melting point of Mg; $\Delta H° = 2.139$ kcal/mol.
1363 K, boiling point of Mg; $\Delta H° = 30.250$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.627 + 0.300\times10^{-3}T - 0.828\times10^{5}T^{-2}$

$H°- H°_{298} = 8.627\times10^{-3}T + 0.150\times10^{-6}T^{2} + 0.828\times10^{2}T^{-1} - 2.863$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf° = -56.355 - 0.770\times10^{-3}T - 1.325\times10^{-6}T^{2} + 30.650T^{-1}$

$\Delta Gf° = -56.355 + 0.770\times10^{-3}T\ln T + 1.325\times10^{-6}T^{2} + 15.325T^{-1} - 26.557\times10^{-3}T$

922-1363 K: $\Delta Hf° = -57.679 - 1.636\times10^{-3}T - 1.011\times10^{-6}T^{2} - 231.050T^{-1}$

$\Delta Gf° = -57.679 + 1.636\times10^{-3}T\ln T + 1.011\times10^{-6}T^{2} - 115.525T^{-1} - 30.590\times10^{-3}T$

1363-2000 K: $\Delta Hf° = -91.537 - 0.595\times10^{-3}T + 0.063\times10^{-6}T^{2} + 32.550T^{-1}$

$\Delta Gf° = -91.537 + 0.595\times10^{-3}T\ln T - 0.063\times10^{-6}T^{2} + 16.275T^{-1} + 3.157\times10^{-3}T$

Source: Data from Chase (26).

$MgF_2(c,l)$
Magnesium Difluoride
[Formation: $Mg(c,l,g) + F_2(g) = MgF_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	14.710	13.680	13.680	0	-268.700	-256.007	187.656
300	14.756	13.771	13.681	.027	-268.698	-255.928	186.441
400	16.440	18.277	14.282	1.598	-268.506	-251.697	137.519
500	17.333	22.050	15.470	3.290	-268.257	-247.526	108.192
600	17.915	25.265	16.842	5.054	-267.989	-243.401	88.658
700	18.350	28.060	18.249	6.868	-267.717	-239.324	74.719
800	18.707	30.534	19.633	8.721	-267.448	-235.290	64.277
900	19.018	32.756	20.969	10.608	-267.183	-231.279	56.162
922	19.080	33.216	21.256	11.027	-267.125	-230.406	54.615
922	19.080	33.216	21.256	11.027	-269.264	-230.406	54.615
1000	19.300	34.775	22.251	12.524	-269.064	-227.134	49.639
1100	19.565	36.627	23.475	14.467	-268.807	-222.956	44.297
1200	19.817	38.340	24.642	16.437	-268.558	-218.800	39.848
1300	20.059	39.936	25.759	18.430	-268.310	-214.651	36.086
1363	20.208	40.889	26.436	19.699	-268.158	-212.075	34.005
1363	20.208	40.889	26.436	19.699	-298.408	-212.075	34.005
1400	20.296	41.431	26.825	20.448	-298.176	-209.735	32.741
1500	20.528	42.839	27.846	22.489	-297.535	-203.442	29.641
1536	20.610	43.327	28.203	23.230	-297.299	-201.186	28.625
1536	22.600	52.363	28.203	37.110	-283.419	-201.186	28.625
1600	22.600	53.286	29.188	38.556	-282.871	-197.770	27.014
1700	22.600	54.656	30.647	40.816	-282.016	-192.477	24.744
1800	22.600	55.948	32.017	43.076	-281.164	-187.235	22.733
1900	22.600	57.170	33.309	45.336	-280.314	-182.038	20.939
2000	22.600	58.329	34.531	47.596	-279.468	-176.888	19.329

Phase changes: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.
1536 K, melting point of MgF_2; ΔH° = 13.880 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1536 K: $Cp^\circ = 17.481 + 2.122\times10^{-3}T - 3.026\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 17.481\times10^{-3}T + 1.061\times10^{-6}T^2 + 3.026\times10^{2}T^{-1} - 6.321$

1536-2000 K: $Cp^\circ = 22.600$
$H^\circ - H^\circ_{298} = 22.600\times10^{-3}T + 2.396$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf^\circ = -270.469 + 3.830\times10^{-3}T - 0.501\times10^{-6}T^2 + 200.200T^{-1}$
$\Delta Gf^\circ = -270.469 - 3.830\times10^{-3}T\ln T + 0.501\times10^{-6}T^2 + 100.100T^{-1} + 69.052\times10^{-3}T$

922-1363 K: $\Delta Hf^\circ = -271.793 + 2.964\times10^{-3}T - 0.187\times10^{-6}T^2 - 61.500T^{-1}$
$\Delta Gf^\circ = -271.793 - 2.964\times10^{-3}T\ln T + 0.187\times10^{-6}T^2 - 30.750T^{-1} + 65.020\times10^{-3}T$

1363-1536 K: $\Delta Hf^\circ = -305.650 + 4.005\times10^{-3}T + 0.887\times10^{-6}T^2 + 202.100T^{-1}$
$\Delta Gf^\circ = -305.650 - 4.005\times10^{-3}T\ln T - 0.887\times10^{-6}T^2 + 101.050T^{-1} + 98.766\times10^{-3}T$

1536-2000 K: $\Delta Hf^\circ = -296.933 + 9.124\times10^{-3}T - 0.174\times10^{-6}T^2 - 100.500T^{-1}$
$\Delta Gf^\circ = -296.933 - 9.124\times10^{-3}T\ln T + 0.174\times10^{-6}T^2 - 50.250T^{-1} + 129.083\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from CODATA (34). Low-temperature heat capacities and entropy at 298 K from Todd (238). High-temperature data based on Naylor (171).

$MgF_2(g)$

Magnesium Difluoride (ideal gas)

[Formation: $Mg(c,l,g) + F_2(g) = MgF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	11.534	61.280	61.280	0	-173.700	-175.199	128.423
300	11.551	61.351	61.281	.021	-173.704	-175.208	127.637
400	12.279	64.782	61.742	1.216	-173.888	-175.681	95.986
500	12.744	67.575	62.639	2.468	-174.079	-176.110	76.977
600	13.045	69.927	63.662	3.759	-174.284	-176.493	64.287
700	13.248	71.954	64.705	5.074	-174.511	-176.843	55.212
800	13.389	73.733	65.726	6.406	-174.763	-177.164	48.398
900	13.490	75.316	66.704	7.751	-175.040	-177.440	43.088
922	13.506	75.642	66.913	8.048	-175.104	-177.502	42.074
922	13.506	75.642	66.913	8.048	-177.243	-177.502	42.074
1000	13.565	76.742	67.638	9.104	-177.484	-177.521	38.797
1100	13.622	78.037	68.525	10.463	-177.811	-177.511	35.268
1200	13.666	79.225	69.368	11.828	-178.167	-177.471	32.321
1300	13.701	80.320	70.169	13.196	-178.544	-177.384	29.821
1363	13.719	80.968	70.653	14.060	-178.797	-177.342	28.435
1363	13.719	80.968	70.653	14.060	-209.047	-177.342	28.435
1400	13.729	81.336	70.930	14.568	-209.056	-176.482	27.550
1500	13.752	82.284	71.656	15.942	-209.082	-174.156	25.374
1600	13.770	83.173	72.349	17.318	-209.109	-171.827	23.470
1700	13.786	84.008	73.010	18.696	-209.136	-169.495	21.790
1800	13.799	84.796	73.643	20.075	-209.165	-167.162	20.296
1900	13.810	85.543	74.251	21.455	-209.195	-164.828	18.959
2000	13.820	86.251	74.832	22.837	-209.227	-162.491	17.756

Phase changes: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.252 + 0.390\times10^{-3}T - 1.631\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.252\times10^{-3}T + 0.195\times10^{-6}T^2 + 1.631\times10^{2}T^{-1} - 4.515$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf^\circ = -173.663 - 0.399\times10^{-3}T - 1.367\times10^{-6}T^2 + 60.700T^{-1}$

$\Delta Gf^\circ = -173.663 + 0.399\times10^{-3}T\ln T + 1.367\times10^{-6}T^2 + 30.350T^{-1} - 8.173\times10^{-3}T$

922-1363 K: $\Delta Hf^\circ = -174.987 - 1.265\times10^{-3}T - 1.053\times10^{-6}T^2 - 201.000T^{-1}$

$\Delta Gf^\circ = -174.987 + 1.265\times10^{-3}T\ln T + 1.053\times10^{-6}T^2 - 100.500T^{-1} - 12.206\times10^{-3}T$

1363-2000 K: $\Delta Hf^\circ = -208.844 - 0.224\times10^{-3}T + 0.021\times10^{-6}T^2 + 62.600T^{-1}$

$\Delta Gf^\circ = -208.844 + 0.224\times10^{-3}T\ln T - 0.021\times10^{-6}T^2 + 31.300T^{-1} + 21.541\times10^{-3}T$

Source: Data from Chase (26).

$(MgF_2)_2(g)$

Dimeric Magnesium Difluoride (ideal gas)

[Formation: $2Mg(c,l,g) + 2F_2(g) = (MgF_2)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	25.693	80.521	80.521	0	-410.700	-401.164	294.057
300	25.749	80.680	80.521	.048	-410.702	-401.103	292.199
400	27.969	88.425	81.563	2.745	-410.763	-397.893	217.396
500	29.195	94.810	83.592	5.609	-410.785	-394.677	172.511
600	29.926	100.203	85.923	8.568	-410.818	-391.446	142.582
700	30.392	104.854	88.303	11.586	-410.884	-388.211	121.203
800	30.706	108.934	90.633	14.641	-410.997	-384.973	105.168
900	30.926	112.564	92.871	17.724	-411.158	-381.697	92.688
922	30.961	113.311	93.350	18.405	-411.199	-380.985	90.307
922	30.961	113.311	93.350	18.405	-415.477	-380.985	90.307
1000	31.086	115.831	95.006	20.825	-415.651	-378.072	82.627
1100	31.206	118.800	97.037	23.939	-415.909	-374.307	74.367
1200	31.298	121.519	98.965	27.065	-416.225	-370.516	67.479
1300	31.370	124.027	100.798	30.198	-416.582	-366.666	61.641
1363	31.407	125.513	101.906	32.176	-416.838	-364.283	58.410
1363	31.407	125.513	101.906	32.176	-477.338	-364.283	58.410
1400	31.428	126.354	102.541	33.338	-477.210	-361.217	56.388
1500	31.474	128.524	104.201	36.484	-476.864	-352.946	51.424
1600	31.513	130.557	105.786	39.633	-476.521	-344.695	47.083
1700	31.544	132.468	107.300	42.786	-476.178	-336.465	43.255
1800	31.571	134.272	108.749	45.942	-475.838	-328.256	39.855
1900	31.594	135.980	110.138	49.100	-475.500	-320.065	36.815
2000	31.613	137.601	111.471	52.260	-475.168	-311.894	34.082

Phase changes: 922 K, melting point of Mg; ΔH° = 2.139 kcal/mol.
1363 K, boiling point of Mg; ΔH° = 30.250 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 30.890 + 0.562\times10^{-3}T - 4.769\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 30.890\times10^{-3}T + 0.281\times10^{-6}T^2 + 4.769\times10^{2}T^{-1} - 10.834$

Formation equations (kcal/mol):

298.15-922 K: $\Delta Hf^\circ = -412.430 + 3.588\times10^{-3}T - 2.843\times10^{-6}T^2 + 272.100T^{-1}$

$\Delta Gf^\circ = -412.430 - 3.588\times10^{-3}T\ln T + 2.843\times10^{-6}T^2 + 136.050T^{-1} + 55.851\times10^{-3}T$

922-1363 K: $\Delta Hf^\circ = -415.077 + 1.856\times10^{-3}T - 2.215\times10^{-6}T^2 - 251.300T^{-1}$

$\Delta Gf^\circ = -415.077 - 1.856\times10^{-3}T\ln T + 2.215\times10^{-6}T^2 - 125.650T^{-1} + 47.786\times10^{-3}T$

1363-2000 K: $\Delta Hf^\circ = -482.792 + 3.938\times10^{-3}T - 0.067\times10^{-6}T^2 + 275.900T^{-1}$

$\Delta Gf^\circ = -482.792 - 3.938\times10^{-3}T\ln T + 0.067\times10^{-6}T^2 + 137.950T^{-1} + 115.279\times10^{-3}T$

Source: Data from Chase (26) who estimated some molecular constants.

MgI(g)

Magnesium Monoiodide (ideal gas)

[Formation: $Mg(c,l,g) + 0.5I_2(s,l,g) = MgI(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.751	65.042	65.042	0	5.900	-7.026	5.150
300	8.755	65.096	65.043	.016	5.893	-7.105	5.176
386.8	8.917	67.343	65.316	.784	5.529	-10.821	6.114
386.8	8.917	67.343	65.316	.784	3.675	-10.821	6.114
400	8.942	67.643	65.388	.902	3.583	-11.314	6.181
458.4	9.010	68.867	65.756	1.426	3.174	-13.462	6.418
458.4	9.010	68.867	65.756	1.426	-1.836	-13.462	6.418
500	9.059	69.652	66.048	1.802	-1.915	-14.513	6.343
600	9.146	71.311	66.789	2.713	-2.118	-17.009	6.195
700	9.219	72.727	67.540	3.631	-2.344	-19.473	6.080
800	9.283	73.962	68.267	4.556	-2.591	-21.906	5.984
900	9.343	75.059	68.961	5.488	-2.863	-24.299	5.901
922	9.356	75.285	69.109	5.694	-2.924	-24.826	5.885
922	9.356	75.285	69.109	5.694	-5.063	-24.826	5.885
1000	9.400	76.046	69.621	6.425	-5.295	-26.493	5.790
1100	9.454	76.945	70.248	7.367	-5.607	-28.603	5.683
1200	9.508	77.770	70.840	8.316	-5.942	-30.680	5.588
1300	9.560	78.533	71.403	9.269	-6.293	-32.715	5.500
1363	9.593	78.986	71.742	9.873	-6.527	-34.008	5.453
1363	9.593	78.986	71.742	9.873	-36.777	-34.008	5.453
1400	9.612	79.243	71.937	10.228	-36.775	-33.934	5.297
1500	9.663	79.908	72.447	11.191	-36.765	-33.734	4.915
1600	9.714	80.534	72.934	12.160	-36.750	-33.532	4.580
1700	9.765	81.124	73.398	13.134	-36.731	-33.332	4.285
1800	9.815	81.684	73.843	14.113	-36.706	-33.133	4.023
1900	9.865	82.216	74.270	15.097	-36.679	-32.934	3.788
2000	9.915	82.723	74.680	16.086	-36.647	-32.737	3.577

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
922 K, melting point of Mg; $\Delta H°$ = 2.139 kcal/mol.
1363 K, boiling point of Mg; $\Delta H°$ = 30.250 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.927 + 0.500\times10^{-3}T - 0.289\times10^{5}T^{-2}$

$H°- H°_{298} = 8.927\times10^{-3}T + 0.250\times10^{-6}T^{2} + 0.289\times10^{2}T^{-1} - 2.781$

MgI(g) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = 6.768 - 2.655\times10^{-3}T - 1.884\times10^{-6}T^2 + 27.000T^{-1}$

$\Delta Gf^\circ = 6.768 + 2.655\times10^{-3}T\ln T + 1.884\times10^{-6}T^2 + 13.500T^{-1} - 62.103\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = 6.041 - 5.857\times10^{-3}T - 1.138\times10^{-6}T^2 + 27.000T^{-1}$

$\Delta Gf^\circ = 6.041 + 5.857\times10^{-3}T\ln T + 1.138\times10^{-6}T^2 + 13.500T^{-1} - 79.011\times10^{-3}T$

458.4-922 K: $\Delta Hf^\circ = -1.316 - 0.687\times10^{-3}T - 1.172\times10^{-6}T^2 + 19.350T^{-1}$

$\Delta Gf^\circ = -1.316 + 0.687\times10^{-3}T\ln T + 1.172\times10^{-6}T^2 + 9.675T^{-1} - 31.280\times10^{-3}T$

922-1363 K: $\Delta Hf^\circ = -2.639 - 1.553\times10^{-3}T - 0.858\times10^{-6}T^2 - 242.350T^{-1}$

$\Delta Gf^\circ = -2.639 + 1.553\times10^{-3}T\ln T + 0.858\times10^{-6}T^2 - 121.175T^{-1} - 35.312\times10^{-3}T$

1363-2000 K: $\Delta Hf^\circ = -36.497 - 0.512\times10^{-3}T + 0.216\times10^{-6}T^2 + 21.250T^{-1}$

$\Delta Gf^\circ = -36.497 + 0.512\times10^{-3}T\ln T - 0.216\times10^{-6}T^2 + 10.625T^{-1} - 1.566\times10^{-3}T$

Source: Data from Chase (26).

$MgI_2(c,l,g)$
Magnesium Diiodide
[Formation: $Mg(c,l,g) + I_2(c,l,g) = MgI_2(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	17.880	31.000	31.000	0	-87.700	-86.338	63.287
300	17.920	31.111	31.001	.033	-87.702	-86.329	62.890
386.8	18.632	35.757	31.565	1.621	-87.850	-85.916	48.544
386.8	18.632	35.757	31.565	1.621	-91.559	-85.916	48.544
400	18.740	36.384	31.714	1.868	-91.649	-85.722	46.836
458.4	19.090	38.963	32.476	2.974	-92.039	-84.829	40.443
458.4	19.090	38.963	32.476	2.974	-102.060	-84.829	40.443
500	19.340	40.632	33.086	3.773	-101.901	-83.270	36.397
600	19.840	44.203	34.648	5.733	-101.504	-79.578	28.986
700	20.250	47.293	36.240	7.737	-101.093	-75.956	23.714
800	20.620	50.022	37.796	9.781	-100.672	-72.396	19.777
900	20.950	52.462	39.291	11.854	-100.254	-68.881	16.726
907	20.970	52.625	39.395	12.000	-100.225	-68.638	16.539
907	24.000	60.343	39.395	19.000	-93.225	-68.638	16.539
922	24.000	60.737	39.739	19.360	-93.115	-68.237	16.175
922	24.000	60.737	39.739	19.360	-95.254	-68.237	16.175
1000	24.000	62.685	41.453	21.232	-94.698	-65.978	14.419
1100	24.000	64.973	43.489	23.632	-94.005	-63.143	12.545
1200	24.000	67.061	45.368	26.032	-93.344	-60.369	10.995
1255	24.000	68.136	46.341	27.352	-92.986	-58.852	10.249
1255	14.860	96.939	46.341	63.500	-56.838	-58.852	10.249
1300	14.863	97.465	48.107	64.165	-56.970	-58.929	9.907
1363	14.867	98.168	50.404	65.102	-57.158	-59.038	9.466
1363	14.867	98.168	50.404	65.102	-87.408	-59.038	9.466
1400	14.869	98.566	51.672	65.652	-87.379	-58.269	9.096
1500	14.873	99.592	54.833	67.139	-87.302	-56.195	8.188
1600	14.877	100.552	57.660	68.627	-87.225	-54.121	7.392
1700	14.880	101.454	60.210	70.115	-87.150	-52.055	6.692
1800	14.883	102.305	62.526	71.603	-87.075	-49.993	6.070
1900	14.885	103.110	64.641	73.091	-87.003	-47.935	5.514
2000	14.887	103.873	66.583	74.580	-86.931	-45.879	5.013

*Data except enthalpy of formation at 298 K and temperature of fusion estimated.

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
907 K, melting point of MgI_2; $\Delta H°$ = 7.000 kcal/mol.
922 K, melting point of Mg; $\Delta H°$ = 2.139 kcal/mol.
1255 K, boiling point of MgI_2 to monomer; $\Delta H°$ = 36.148 kcal/mol.
1363 K, boiling point of Mg; $\Delta H°$ = 30.250 kcal/mol.

MgI_2(c,l,g) - Continued

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-907 K: $Cp^\circ = 18.189 + 3.214\times10^{-3}T - 1.127\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 18.189\times10^{-3}T + 1.607\times10^{-6}T^2 + 1.127\times10^{2}T^{-1} - 5.944$

907-1255 K: $Cp^\circ = 24.000$

$H^\circ - H^\circ_{298} = 24.000\times10^{-3}T - 2.768$

1255-2000 K: $Cp^\circ = 14.103 + 0.356\times10^{-3}T + 4.878\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.103\times10^{-3}T + 0.178\times10^{-6}T^2 - 4.878\times10^{2}T^{-1} + 45.909$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -88.009 + 0.169\times10^{-3}T - 1.273\times10^{-6}T^2 + 110.800T^{-1}$

$\Delta Gf^\circ = -88.009 - 0.169\times10^{-3}T\ln T + 1.273\times10^{-6}T^2 + 55.400T^{-1} + 5.564\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -89.464 - 6.235\times10^{-3}T + 0.219\times10^{-6}T^2 + 110.800T^{-1}$

$\Delta Gf^\circ = -89.464 + 6.235\times10^{-3}T\ln T - 0.219\times10^{-6}T^2 + 55.400T^{-1} - 28.251\times10^{-3}T$

458.4-907 K: $\Delta Hf^\circ = -104.177 + 4.105\times10^{-3}T + 0.151\times10^{-6}T^2 + 95.500T^{-1}$

$\Delta Gf^\circ = -104.177 - 4.105\times10^{-3}T\ln T - 0.151\times10^{-6}T^2 + 47.750T^{-1} + 67.212\times10^{-3}T$

907-922 K: $\Delta Hf^\circ = -101.002 + 9.916\times10^{-3}T - 1.456\times10^{-6}T^2 - 17.200T^{-1}$

$\Delta Gf^\circ = -101.002 - 9.916\times10^{-3}T\ln T + 1.456\times10^{-6}T^2 - 8.600T^{-1} + 101.895\times10^{-3}T$

922-1255 K: $\Delta Hf^\circ = -102.325 + 9.050\times10^{-3}T - 1.142\times10^{-6}T^2 - 278.900T^{-1}$

$\Delta Gf^\circ = -102.325 - 9.050\times10^{-3}T\ln T + 1.142\times10^{-6}T^2 - 139.450T^{-1} + 97.862\times10^{-3}T$

1255-1363 K: $\Delta Hf^\circ = -53.648 - 0.847\times10^{-3}T - 0.964\times10^{-6}T^2 - 766.700T^{-1}$

$\Delta Gf^\circ = -53.648 + 0.847\times10^{-3}T\ln T + 0.964\times10^{-6}T^2 - 383.350T^{-1} - 11.160\times10^{-3}T$

1363-2000 K: $\Delta Hf^\circ = -87.506 + 0.194\times10^{-3}T + 0.110\times10^{-6}T^2 - 503.100T^{-1}$

$\Delta Gf^\circ = -87.506 - 0.194\times10^{-3}T\ln T - 0.110\times10^{-6}T^2 - 251.550T^{-1} + 22.587\times10^{-3}T$

Source: Data from Chase (26) who estimated all data except enthalpy of formation at 298 K and temperature of fusion.

$MgI_2(g)$

Magnesium Diiodide (ideal gas)

[Formation: $Mg(c,l,g) + I_2(c,l,g) = MgI_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	14.250	75.854	75.854	0	-38.300	-50.311	36.879
300	14.257	75.943	75.856	.026	-38.309	-50.385	36.705
386.8	14.478	79.597	76.301	1.275	-38.796	-53.820	30.409
386.8	14.478	79.597	76.301	1.275	-42.505	-53.820	30.409
400	14.512	80.083	76.418	1.466	-42.651	-54.203	29.615
458.4	14.589	82.067	77.013	2.317	-43.295	-55.845	26.625
458.4	14.589	82.067	77.013	2.317	-53.316	-55.845	26.625
500	14.644	83.337	77.487	2.925	-53.349	-56.071	24.508
600	14.720	86.015	78.693	4.393	-53.444	-56.605	20.618
700	14.767	88.288	79.905	5.868	-53.562	-57.122	17.834
800	14.798	90.262	81.079	7.346	-53.707	-57.623	15.742
900	14.820	92.006	82.198	8.827	-53.881	-58.097	14.108
922	14.824	92.364	82.437	9.153	-53.922	-58.204	13.796
922	14.824	92.364	82.437	9.153	-56.061	-58.204	13.796
1000	14.836	93.568	83.258	10.310	-56.220	-58.383	12.759
1100	14.847	94.983	84.261	11.794	-56.443	-58.592	11.641
1200	14.856	96.275	85.208	13.280	-56.696	-58.778	10.705
1300	14.863	97.465	86.107	14.765	-56.970	-58.929	9.907
1363	14.867	98.168	86.648	15.702	-57.158	-59.038	9.466
1363	14.867	98.168	86.648	15.702	-87.408	-59.038	9.466
1400	14.869	98.566	86.957	16.252	-87.379	-58.269	9.096
1500	14.873	99.592	87.766	17.739	-87.302	-56.195	8.188
1600	14.877	100.552	88.535	19.227	-87.225	-54.121	7.392
1700	14.880	101.454	89.269	20.715	-87.150	-52.055	6.692
1800	14.883	102.305	89.970	22.203	-87.075	-49.993	6.070
1900	14.885	103.110	90.641	23.691	-87.003	-47.935	5.514
2000	14.887	103.873	91.283	25.180	-86.931	-45.879	5.013

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
922 K, melting point of Mg; $\Delta H°$ = 2.139 kcal/mol.
1363 K, boiling point of Mg; $\Delta H°$ = 30.250 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 14.847 + 0.034\times10^{-3}T - 0.540\times10^{5}T^{-2}$

$H°- H°_{298} = 14.847\times10^{-3}T + 0.017\times10^{-6}T^{2} + 0.540\times10^{2}T^{-1} - 4.609$

$MgI_2(g)$ - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -37.274 - 3.173\times10^{-3}T - 2.863\times10^{-6}T^2 + 52.100T^{-1}$

$\Delta Gf^\circ = -37.274 + 3.173\times10^{-3}T\ln T + 2.863\times10^{-6}T^2 + 26.050T^{-1} - 62.952\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -38.729 - 9.577\times10^{-3}T - 1.371\times10^{-6}T^2 + 52.100T^{-1}$

$\Delta Gf^\circ = -38.729 + 9.577\times10^{-3}T\ln T + 1.371\times10^{-6}T^2 + 26.050T^{-1} - 96.767\times10^{-3}T$

458.4-922 K: $\Delta Hf^\circ = -53.443 + 0.763\times10^{-3}T - 1.439\times10^{-6}T^2 + 36.800T^{-1}$

$\Delta Gf^\circ = -53.443 - 0.763\times10^{-3}T\ln T + 1.439\times10^{-6}T^2 + 18.400T^{-1} - 1.304\times10^{-3}T$

922-1363 K: $\Delta Hf^\circ = -54.766 - 0.103\times10^{-3}T - 1.125\times10^{-6}T^2 - 224.900T^{-1}$

$\Delta Gf^\circ = -54.766 + 0.103\times10^{-3}T\ln T + 1.125\times10^{-6}T^2 - 112.450T^{-1} - 5.337\times10^{-3}T$

1363-2000 K: $\Delta Hf^\circ = -88.624 + 0.938\times10^{-3}T - 0.051\times10^{-6}T^2 + 38.700T^{-1}$

$\Delta Gf^\circ = -88.624 - 0.938\times10^{-3}T\ln T + 0.051\times10^{-6}T^2 + 19.350T^{-1} + 28.410\times10^{-3}T$

Source: Data from Chase (26) who estimated most molecular constants.

$MnCl_2(c,l)$

Manganese Dichloride

[Formation: $Mn(c) + Cl_2(g) = MnCl_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	17.450	28.260	28.260	0	-115.030	-105.286	77.176
300	17.472	28.368	28.261	.032	-115.025	-105.226	76.656
400	18.387	33.532	28.957	1.830	-114.709	-102.008	55.734
500	19.004	37.705	30.303	3.701	-114.389	-98.867	43.214
600	19.506	41.215	31.837	5.627	-114.074	-95.793	34.892
700	19.955	44.256	33.399	7.600	-113.761	-92.775	28.965
800	20.375	46.948	34.927	9.617	-113.448	-89.800	24.532
900	20.778	49.371	36.400	11.674	-113.131	-86.864	21.093
923	20.869	49.897	36.730	12.153	-113.057	-86.194	20.409
923	22.540	59.659	36.730	21.163	-104.047	-86.194	20.409
980	22.540	61.010	38.103	22.448	-103.772	-85.097	18.977
980	22.540	61.010	38.103	22.448	-104.304	-85.097	18.977
1000	22.540	61.465	38.566	22.899	-104.212	-84.709	18.513
1100	22.540	63.613	40.747	25.153	-103.760	-82.772	16.445
1200	22.540	65.574	42.735	27.407	-103.322	-80.892	14.732
1300	22.540	67.378	44.562	29.661	-102.896	-79.041	13.288
1360	22.540	68.396	45.592	31.013	-102.647	-77.937	12.524
1360	22.540	68.396	45.592	31.013	-103.154	-77.937	12.524
1400	22.540	69.049	46.253	31.915	-103.028	-77.199	12.051

Phase changes: 923 K, melting point of $MnCl_2$; ΔH° = 9.010 kcal/mol.
980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.
1360 K, β - γ transition point of Mn; ΔH° = 0.507 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-923 K: $Cp^\circ = 17.638 + 3.640\times10^{-3}T - 1.132\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 17.638\times10^{-3}T + 1.820\times10^{-6}T^2 + 1.132\times10^{2}T^{-1} - 5.800$

923-1400 K: $Cp^\circ = 22.540$

$H^\circ - H^\circ_{298} = 22.540\times10^{-3}T + 0.359$

Formation equations (kcal/mol):

298.15-923 K: $\Delta Hf^\circ = -116.017 + 3.173\times10^{-3}T + 0.025\times10^{-6}T^2 + 11.500T^{-1}$

$\Delta Gf^\circ = -116.017 - 3.173\times10^{-3}T\ln T - 0.025\times10^{-6}T^2 + 5.750T^{-1} + 54.011\times10^{-3}T$

923-980 K: $\Delta Hf^\circ = -109.858 + 8.075\times10^{-3}T - 1.795\times10^{-6}T^2 - 101.700T^{-1}$

$\Delta Gf^\circ = -109.858 - 8.075\times10^{-3}T\ln T + 1.795\times10^{-6}T^2 - 50.850T^{-1} + 79.194\times10^{-3}T$

980-1360 K: $\Delta Hf^\circ = -109.439 + 5.894\times10^{-3}T - 0.652\times10^{-6}T^2 - 14.900T^{-1}$

$\Delta Gf^\circ = -109.439 - 5.894\times10^{-3}T\ln T + 0.652\times10^{-6}T^2 - 7.450T^{-1} + 64.820\times10^{-3}T$

1360-1400 K: $\Delta Hf^\circ = -109.412 + 6.123\times10^{-3}T - 1.088\times10^{-6}T^2 - 68.300T^{-1}$

$\Delta Gf^\circ = -109.412 - 6.123\times10^{-3}T\ln T + 1.088\times10^{-6}T^2 - 34.150T^{-1} + 65.874\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (253). Low-temperature heat capacities and entropy at 298 K from Chisholm (29). High-temperature data based on Moore (160).

$MnF_2(c)$
Manganese Difluoride
[Formation: $Mn(c) + F_2(g) = MnF_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	16.202	22.250	22.250	0	-203.000	-192.910	141.405
300	16.231	22.350	22.250	.030	-202.996	-192.847	140.487
400	17.426	27.198	22.903	1.718	-202.729	-189.504	103.539
500	18.206	31.175	24.171	3.502	-202.447	-186.228	81.399
600	18.805	34.549	25.627	5.353	-202.168	-183.012	66.661
700	19.319	37.487	27.116	7.260	-201.891	-179.845	56.149
800*	19.801	40.099	28.579	9.216	-201.615	-176.717	48.276
900	20.275	42.458	29.991	11.220	-201.332	-173.620	42.160
980	20.664	44.202	31.081	12.858	-201.098	-171.164	38.171
980	20.664	44.202	31.081	12.858	-201.630	-171.164	38.171
1000	20.761	44.620	31.348	13.272	-201.572	-170.547	37.273
1023	20.875	45.093	31.652	13.750	-201.505	-169.835	36.282
1023	20.875	45.582	31.652	14.250	-201.005	-169.835	36.282
1100	21.267	47.111	32.681	15.873	-200.762	-167.488	33.276
1200	21.801	48.984	33.962	18.026	-200.416	-164.487	29.957

*Data above 770 K extrapolated.

Phase changes: 980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.
1023 K, α - β transition point of MnF_2; ΔH° = 0.500 kcal/mol.
1173 ± 20 K, melting point of MnF_2; ΔH° = approximately 7 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1023 K:
$$Cp^\circ = 16.809 + 4.074\times10^{-3}T - 1.619\times10^{5}T^{-2}$$
$$H^\circ - H^\circ_{298} = 16.809\times10^{-3}T + 2.037\times10^{-5}T^2 + 1.619\times10^{2}T^{-1} - 5.736$$

1023-1200 K:
$$Cp^\circ = 15.656 + 5.108\times10^{-3}T$$
$$H^\circ - H^\circ_{298} = 15.656\times10^{-3}T + 2.554\times10^{-6}T^2 - 4.439$$

Formation equations (kcal/mol):

298.15-980 K:
$$\Delta Hf^\circ = -203.902 + 2.663\times10^{-3}T + 0.156\times10^{-6}T^2 + 28.000T^{-1}$$
$$\Delta Gf^\circ = -203.902 - 2.663\times10^{-3}T\ln T - 0.156\times10^{-6}T^2 + 14.000T^{-1} + 51.929\times10^{-3}T$$

980-1023 K:
$$\Delta Hf^\circ = -203.483 + 0.482\times10^{-3}T + 1.299\times10^{-6}T^2 + 114.800T^{-1}$$
$$\Delta Gf^\circ = -203.483 - 0.482\times10^{-3}T\ln T - 1.299\times10^{-6}T^2 + 57.400T^{-1} + 37.555\times10^{-3}T$$

1023-1200 K:
$$\Delta Hf^\circ = -202.186 - 0.671\times10^{-3}T + 1.816\times10^{-6}T^2 - 47.100T^{-1}$$
$$\Delta Gf^\circ = -202.186 + 0.671\times10^{-3}T\ln T - 1.816\times10^{-6}T^2 - 23.550T^{-1} + 28.903\times10^{-3}T$$

Sources: Enthalpy of formation at 298 K from Ehlert (76). Low-temperature heat capacities and entropy at 298 K from Stout (226). High-temperature data to 770 K based on Ehlert (76). Data above 770 K extrapolated. Temperatures and enthalpies of transition and fusion from Rimai (197).

$MnF_2(g)$

Manganese Difluoride (ideal gas)

[Formation: $Mn(c) + F_2(g) = MnF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.650	65.096	65.096	0	-127.000	-129.684	95.060
300	12.668	65.174	65.097	.023	-127.003	-129.702	94.486
400	13.409	68.929	65.604	1.330	-127.117	-130.585	71.347
500	13.858	71.973	66.581	2.696	-127.253	-131.433	57.449
600	14.140	74.526	67.699	4.096	-127.425	-132.256	48.173
700	14.324	76.721	68.835	5.520	-127.631	-133.048	41.539
800	14.451	78.642	69.943	6.959	-127.872	-133.808	36.554
900	14.540	80.350	71.007	8.409	-128.143	-134.534	32.669
980	14.593	81.590	71.820	9.575	-128.381	-135.088	30.126
980	14.593	81.590	71.820	9.575	-128.913	-135.088	30.126
1000	14.606	81.885	72.018	9.867	-128.977	-135.217	29.551
1100	14.656	83.280	72.980	11.330	-129.305	-135.817	26.984
1200	14.694	84.557	73.893	12.797	-129.645	-136.403	24.842

Phase change: 980 K, α - β transition point of Mn; ΔH° = 0.532 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp^\circ = 14.138 + 0.624\times10^{-3}T - 1.488\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.138\times10^{-3}T + 0.312\times10^{-6}T^2 + 1.488\times10^{2}T^{-1} - 4.742$

Formation equations (kcal/mol):

298.15-980 K: $\Delta Hf^\circ = -126.908 - 0.008\times10^{-3}T - 1.569\times10^{-6}T^2 + 14.900T^{-1}$

$\Delta Gf^\circ = -126.908 + 0.008\times10^{-3}T\ln T + 1.569\times10^{-6}T^2 + 7.450T^{-1} - 9.908\times10^{-3}T$

980-1200 K: $\Delta Hf^\circ = -126.489 - 2.189\times10^{-3}T - 0.426\times10^{-6}T^2 + 101.700T^{-1}$

$\Delta Gf^\circ = -126.489 + 2.189\times10^{-3}T\ln T + 0.426\times10^{-6}T^2 + 50.850T^{-1} - 24.283\times10^{-3}T$

Source: All data from Ehlert (76).

MoBr(g)
Molybdenum Monobromide (ideal gas)
[Formation: Mo(c) + 0.5Br_2(l,g) = MoBr(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H°_{298})/T	H°- H°_{298}	ΔHf°	ΔGf°	
298.15*	8.652	64.380	64.380	0	109.300	97.571	-71.520
300	8.656	64.434	64.381	.016	109.289	97.498	-71.026
332.6	8.701	65.329	64.431	.299	109.089	96.227	-63.229
332.6	8.701	65.329	64.431	.299	105.556	96.227	-63.229
400	8.794	66.945	64.722	.889	105.454	94.344	-51.547
500	8.866	68.916	65.370	1.773	105.290	91.587	-40.032
600	8.910	70.537	66.100	2.662	105.110	88.862	-32.368
700	8.941	71.913	66.836	3.554	104.918	86.169	-26.903
800	8.964	73.108	67.547	4.449	104.716	83.504	-22.812
900	8.982	74.165	68.224	5.347	104.506	80.866	-19.637
1000	8.998	75.112	68.866	6.246	104.285	78.250	-17.101
1100	9.012	75.971	69.475	7.146	104.050	75.657	-15.031
1200	9.026	76.755	70.048	8.048	103.803	73.089	-13.311
1300	9.039	77.478	70.592	8.952	103.539	70.540	-11.859
1400	9.052	78.149	71.109	9.856	103.259	68.011	-10.617
1500	9.068	78.774	71.599	10.762	102.962	65.503	-9.544
1600	9.087	79.360	72.066	11.670	102.649	63.017	-8.608
1700	9.110	79.911	72.511	12.580	102.318	60.550	-7.784
1800	9.141	80.433	72.937	13.492	101.966	58.103	-7.055
1900	9.180	80.928	73.345	14.408	101.593	55.677	-6.404
2000	9.231	81.400	73.736	15.329	101.199	53.270	-5.821

*Data estimated.

Phase change: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.911 + 0.118\times10^{-3}T - 0.262\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.911\times10^{-3}T + 0.059\times10^{-6}T^2 + 0.262\times10^{2}T^{-1} - 2.750$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = 110.454 - 4.511\times10^{-3}T - 1.076\times10^{-6}T^2 + 85.400T^{-1}$

$\Delta Gf^\circ = 110.454 + 4.511\times10^{-3}T\ln T + 1.076\times10^{-6}T^2 + 42.700T^{-1} - 69.718\times10^{-3}T$

332.6-2000 K: $\Delta Hf^\circ = 105.454 + 0.069\times10^{-3}T - 1.154\times10^{-6}T^2 + 69.700T^{-1}$

$\Delta Gf^\circ = 105.454 - 0.069\times10^{-3}T\ln T + 1.154\times10^{-6}T^2 + 34.850T^{-1} - 28.040\times10^{-3}T$

Source: Data are estimations from JANAF (61).

$MoBr_2$(c)

Molybdenum Dibromide

[Formation: Mo(c) + Br_2(l,g) = $MoBr_2$(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	19.045	29.800	29.800	0	-48.500	-44.496	32.616
300	19.050	29.918	29.801	.035	-48.509	-44.471	32.397
332.6	19.131	31.887	29.911	.657	-48.663	-44.025	28.928
332.6	19.131	31.887	29.911	.657	-55.728	-44.025	28.928
400	19.300	35.432	30.549	1.953	-55.420	-41.685	22.775
500	19.550	39.766	31.976	3.895	-54.967	-38.304	16.742
600	19.800	43.352	33.580	5.863	-54.512	-35.013	12.753
700	20.050	46.423	35.202	7.855	-54.050	-31.800	9.928
800	20.300	49.117	36.776	9.873	-53.576	-28.653	7.827
900	20.550	51.522	38.283	11.915	-53.092	-25.567	6.209
1000	20.800	53.701	39.718	13.983	-52.594	-22.537	4.925
1100	21.050	55.695	41.081	16.075	-52.088	-19.555	3.885
1200	21.300	57.537	42.376	18.193	-51.571	-16.619	3.027
1300	21.550	59.252	43.610	20.335	-51.049	-13.729	2.308
1400	21.800	60.858	44.784	22.503	-50.518	-10.876	1.698

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
1353 ± 30 K, decomposition point of $MoBr_2$.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1400 K: $Cp^\circ = 18.293 + 2.508\times10^{-3}T + 0.004\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 18.293\times10^{-3}T + 1.254\times10^{-6}T^2 - 0.004\times10^{2}T^{-1} - 5.564$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -47.467 - 4.175\times10^{-3}T + 0.169\times10^{-6}T^2 + 58.800T^{-1}$

$\Delta Gf^\circ = -47.467 + 4.175\times10^{-3}T\ln T - 0.169\times10^{-6}T^2 + 29.400T^{-1} - 14.102\times10^{-3}T$

332.6-1400 K: $\Delta Hf^\circ = -57.468 + 4.986\times10^{-3}T + 0.014\times10^{-6}T^2 + 27.400T^{-1}$

$\Delta Gf^\circ = -57.468 - 4.986\times10^{-3}T\ln T - 0.014\times10^{-6}T^2 + 13.700T^{-1} + 69.253\times10^{-3}T$

Source: Data from JANAF (61). All are estimations except enthalpy of formation at 298 K.

$MoBr_2(g)$
Molybdenum Dibromide (ideal gas)
[Formation: $Mo(c) + Br_2(l,g) = MoBr_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	16.561	76.686	76.686	0	40.000	30.025	-22.008
300	16.568	76.788	76.686	.031	39.987	29.964	-21.828
332.6	16.653	78.501	76.780	.572	39.752	28.886	-18.981
332.6	16.653	78.501	76.780	.572	32.687	28.886	-18.981
400	16.828	81.596	77.339	1.703	32.830	28.100	-15.353
500	16.871	85.359	78.581	3.389	33.027	26.894	-11.755
600	16.780	88.429	79.976	5.072	33.197	25.650	-9.343
700	16.619	91.004	81.371	6.743	33.338	24.382	-7.612
800	16.437	93.211	82.716	8.396	33.447	23.095	-6.309
900	16.257	95.137	83.993	10.030	33.523	21.794	-5.292
1000	16.093	96.841	85.193	11.648	33.571	20.488	-4.478
1100	15.948	98.368	86.323	13.249	33.586	19.178	-3.810
1200	15.823	99.750	87.385	14.838	33.574	17.871	-3.255
1300	15.716	101.012	88.385	16.415	33.531	16.563	-2.785
1400	15.625	102.173	89.329	17.982	33.461	15.262	-2.383
1500	15.548	103.249	90.222	19.540	33.362	13.963	-2.034
1600	15.484	104.250	91.067	21.092	33.239	12.676	-1.731
1700	15.430	105.187	91.871	22.637	33.087	11.393	-1.465
1800	15.387	106.068	92.636	24.178	32.909	10.123	-1.229
1900	15.352	106.899	93.365	25.715	32.701	8.864	-1.020
2000	15.326	107.685	94.061	27.249	32.463	7.615	-.832

*Data estimated.

Phase change: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 17.768 - 1.450\times10^{-3}T - 0.689\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 17.768\times10^{-3}T - 0.725\times10^{-6}T^2 + 0.689\times10^{2}T^{-1} - 5.464$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = 41.133 - 4.700\times10^{-3}T - 1.810\times10^{-6}T^2 + 128.100T^{-1}$

$\Delta Gf^\circ = 41.133 + 4.700\times10^{-3}T\ln T + 1.810\times10^{-6}T^2 + 64.050T^{-1} - 65.294\times10^{-3}T$

332.6-2000 K: $\Delta Hf^\circ = 31.132 + 4.461\times10^{-3}T - 1.965\times10^{-6}T^2 + 96.700T^{-1}$

$\Delta Gf^\circ = 31.132 - 4.461\times10^{-3}T\ln T + 1.965\times10^{-6}T^2 + 48.350T^{-1} + 18.061\times10^{-3}T$

Source: Data are estimations from JANAF (61).

$MoBr_3(c)$

Molybdenum Tribromide

[Formation: $Mo(c) + 1.5Br_2(l,g) = MoBr_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	25.184	41.700	41.700	0	-67.800	-61.921	45.389
300	25.190	41.856	41.700	.047	-67.814	-61.884	45.082
332.6	25.304	44.460	41.845	.870	-68.061	-61.227	40.231
332.6	25.304	44.460	41.845	.870	-78.659	-61.227	40.231
400	25.540	49.150	42.693	2.583	-78.228	-57.740	31.547
500	25.890	54.887	44.577	5.155	-77.586	-52.692	23.031
600	26.240	59.638	46.703	7.761	-76.937	-47.774	17.401
700	26.590	63.710	48.849	10.403	-76.271	-42.966	13.414
800	26.940	67.283	50.934	13.079	-75.587	-38.254	10.450
900	27.290	70.476	52.930	15.791	-74.882	-33.630	8.166
1000	27.640	73.370	54.833	18.537	-74.156	-29.087	6.357
1100	27.990	76.021	56.640	21.319	-73.411	-24.615	4.890

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
1087 ± 20 K, decomposition point of $MoBr_3$.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1100 K: $Cp^\circ = 24.154 + 3.482\times10^{-3}T - 0.008\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 24.154\times10^{-3}T + 1.741\times10^{-6}T^2 + 0.008\times10^{2}T^{-1} - 7.359$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -65.870 - 7.360\times10^{-3}T + 0.706\times10^{-6}T^2 + 60.000T^{-1}$

$\Delta Gf^\circ = -65.870 + 7.360\times10^{-3}T\ln T - 0.706\times10^{-6}T^2 + 30.000T^{-1} - 28.814\times10^{-3}T$

332.6-1100 K: $\Delta Hf^\circ = -80.870 + 6.382\times10^{-3}T + 0.473\times10^{-6}T^2 + 12.900T^{-1}$

$\Delta Gf^\circ = -80.870 - 6.382\times10^{-3}T\ln T - 0.473\times10^{-6}T^2 + 6.450T^{-1} + 96.219\times10^{-3}T$

Source: Data from JANAF (61). All are estimations except enthalpy of formation at 298 K.

$MoBr_3(g)$
Molybdenum Tribromide (ideal gas)
[Formation: $Mo(c) + 1.5Br_2(l,g) = MoBr_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	19.185	89.599	89.599	0	-2.000	-10.402	7.625
300	19.193	89.717	89.600	.035	-2.026	-10.454	7.616
332.6	19.287	91.702	89.711	.662	-2.469	-11.347	7.456
332.6	19.287	91.702	89.711	.662	-13.067	-11.347	7.456
400	19.481	95.284	90.356	1.971	-13.039	-11.006	6.013
500	19.626	99.648	91.794	3.927	-13.013	-10.500	4.590
600	19.726	103.235	93.410	5.895	-13.003	-9.998	3.642
700	19.817	106.283	95.037	7.872	-13.002	-9.498	2.965
800	19.915	108.936	96.612	9.859	-13.006	-8.996	2.458
900	20.021	111.287	98.115	11.855	-13.018	-8.496	2.063
1000	20.130	113.402	99.539	13.863	-13.030	-7.993	1.747
1100	20.237	115.326	100.889	15.881	-13.049	-7.488	1.488
1200	20.339	117.091	102.166	17.910	-13.073	-6.980	1.271
1300	20.433	118.723	103.378	19.949	-13.106	-6.472	1.088
1400	20.517	120.240	104.529	21.996	-13.149	-5.959	.930
1500	20.593	121.658	105.623	24.052	-13.204	-5.444	.793
1600	20.661	122.990	106.668	26.115	-13.271	-4.924	.673
1700	20.723	124.244	107.665	28.184	-13.354	-4.401	.566
1800	20.780	125.430	108.619	30.259	-13.453	-3.871	.470
1900	20.835	126.555	109.534	32.340	-13.573	-3.333	.383
2000	20.888	127.625	110.412	34.426	-13.716	-2.793	.305

*Data estimated.

Phase change: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.338 + 0.832\times10^{-3}T - 0.357\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.338\times10^{-3}T + 0.416\times10^{-6}T^2 + 0.357\times10^{2}T^{-1} - 5.922$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = 1.367 - 12.176\times10^{-3}T - 0.619\times10^{-6}T^2 + 94.900T^{-1}$

$\Delta Gf^\circ = 1.367 + 12.176\times10^{-3}T\ln T + 0.619\times10^{-6}T^2 + 47.450T^{-1} - 109.562\times10^{-3}T$

332.6-2000 K: $\Delta Hf^\circ = -13.634 + 1.566\times10^{-3}T - 0.852\times10^{-6}T^2 + 47.800T^{-1}$

$\Delta Gf^\circ = -13.634 - 1.566\times10^{-3}T\ln T + 0.852\times10^{-6}T^2 + 23.900T^{-1} + 15.470\times10^{-3}T$

Source: Data are estimations from JANAF (61).

$MoBr_4$(c)
Molybdenum Tetrabromide
[Formation: Mo(c) + $2Br_2$(l,g) = $MoBr_4$(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	31.800	50.000	50.000	0	-72.700	-63.872	46.819
300	31.810	50.197	50.000	.059	-72.718	-63.817	46.490
332.6	31.970	53.487	50.184	1.099	-73.043	-62.833	41.287
332.6	31.970	53.487	50.184	1.099	-87.173	-62.833	41.287
400	32.300	59.417	51.255	3.265	-86.583	-57.963	31.669
500	32.700	66.666	53.638	6.514	-85.705	-50.910	22.252

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.
413 ± 20 K, decomposition point of $MoBr_4$.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-500 K: $Cp° = 30.403 + 4.684\times10^{-3}T$

$H°-H°_{298} = 30.403\times10^{-3}T + 2.342\times10^{-6}T^2 - 9.273$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -69.991 - 10.156\times10^{-3}T + 1.357\times10^{-6}T^2 + 59.200T^{-1}$

$\Delta Gf° = -69.991 + 10.156\times10^{-3}T\ln T - 1.357\times10^{-6}T^2 + 29.600T^{-1} - 37.271\times10^{-3}T$

332.6-500 K: $\Delta Hf° = -89.992 + 8.166\times10^{-3}T + 1.047\times10^{-6}T^2 - 3.600T^{-1}$

$\Delta Gf° = -89.992 - 8.166\times10^{-3}T\ln T - 1.047\times10^{-6}T^2 - 1.800T^{-1} + 129.440\times10^{-3}T$

Source: Data from JANAF (61) who estimated all except enthalpy of formation at 298 K.

$MoBr_4(g)$

Molybdenum Tetrabromide (ideal gas)

[Formation: $Mo(c) + 2Br_2(l,g) = MoBr_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	24.590	100.091	100.091	0	-40.900	-47.007	34.457
300	24.604	100.243	100.091	.046	-40.931	-47.043	34.271
332.6	24.771	102.790	100.232	.851	-41.491	-47.679	31.329
332.6	24.771	102.790	100.232	.851	-55.621	-47.679	31.329
400	25.116	107.401	101.063	2.535	-55.513	-46.087	25.180
500	25.366	113.035	102.915	5.060	-55.359	-43.749	19.122
600	25.506	117.673	105.000	7.604	-55.216	-41.439	15.094
700	25.591	121.612	107.098	10.160	-55.083	-39.153	12.224
800	25.647	125.033	109.131	12.722	-54.960	-36.885	10.076
900	25.686	128.056	111.069	15.288	-54.851	-34.634	8.410
1000	25.714	130.764	112.905	17.859	-54.750	-32.394	7.080
1100	25.734	133.216	114.642	20.431	-54.666	-30.162	5.993
1200	25.750	135.456	116.285	23.005	-54.596	-27.937	5.088
1300	25.763	137.517	117.839	25.581	-54.545	-25.717	4.323
1400	25.773	139.427	119.314	28.158	-54.511	-23.500	3.668
1500	25.781	141.205	120.715	30.735	-54.499	-21.288	3.102
1600	25.788	142.870	122.049	33.314	-54.504	-19.072	2.605
1700	25.796	144.433	123.319	35.893	-54.532	-16.858	2.167
1800	25.803	145.908	124.534	38.473	-54.582	-14.640	1.778
1900	25.811	147.303	125.696	41.054	-54.658	-12.415	1.428
2000	25.822	148.627	126.810	43.635	-54.763	-10.193	1.114

*Data except enthalpy of formation at 298 K estimated.

Phase change: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 25.775 + 0.038\times10^{-3}T - 1.064\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.775\times10^{-3}T + 0.019\times10^{-6}T^2 + 1.064\times10^{2}T^{-1} - 8.043$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -36.962 - 14.784\times10^{-3}T - 0.966\times10^{-6}T^2 + 165.600T^{-1}$

$\Delta Gf^\circ = -36.962 + 14.784\times10^{-3}T\ln T + 0.966\times10^{-6}T^2 + 82.800T^{-1} - 119.145\times10^{-3}T$

332.6-2000 K: $\Delta Hf^\circ = -56.962 + 3.538\times10^{-3}T - 1.276\times10^{-6}T^2 + 102.800T^{-1}$

$\Delta Gf^\circ = -56.962 - 3.538\times10^{-3}T\ln T + 1.276\times10^{-6}T^2 + 51.400T^{-1} + 47.565\times10^{-3}T$

Source: Data from JANAF (61). All are estimations except enthalpy of formation at 298 K.

$MoCl_3(c)$
Molybdenum Trichloride
[Formation: $Mo(c) + 1.5Cl_2(g) = MoCl_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	22.658	28.240	28.240	0	-94.000	-76.545	56.108
300*	22.697	28.380	28.240	.042	-93.992	-76.437	55.683
400	24.321	35.152	29.152	2.400	-93.465	-70.662	38.607
500	25.359	40.698	30.924	4.887	-92.865	-65.028	28.423
600	26.099	45.391	32.954	7.462	-92.219	-59.522	21.681
700	26.666	49.458	35.028	10.101	-91.534	-54.125	16.899
800	27.120	53.049	37.060	12.791	-90.822	-48.831	13.340
900	27.498	56.266	39.018	15.523	-90.083	-43.625	10.593
1000	27.818	59.180	40.891	18.289	-89.328	-38.505	8.415

*Data above 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 24.694 + 3.518\times10^{-3}T - 2.743\times10^{5}T^{-2}$

$H°- H°_{298} = 24.694\times10^{-3}T + 1.759\times10^{-6}T^{2} + 2.743\times10^{2}T^{-1} - 8.439$

Formation equations (kcal/mol):

298.15-1000 K: $\Delta Hf° = -96.924 + 7.076\times10^{-3}T + 0.442\times10^{-6}T^{2} + 231.050T^{-1}$

$\Delta Gf° = -96.924 - 7.076\times10^{-3}T\ln T - 0.442\times10^{-6}T^{2} + 115.525T^{-1} + 107.504\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Shchukarev (210). Low-temperature heat capacities and entropy at 298 K from Kiwia (130). High-temperature data estimated.

$MoCl_4(c)$

Molybdenum Tetrachloride

[Formation: $Mo(c) + 2Cl_2(g) = MoCl_4(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	28.280	37.580	37.580	0	-114.000	-91.385	66.986
300*	28.323	37.755	37.582	.052	-113.989	-91.246	66.472
400	29.774	46.134	38.714	2.968	-113.320	-83.764	45.766
500	30.570	52.867	40.893	5.987	-112.614	-76.454	33.418
600	31.142	58.498	43.370	9.077	-111.887	-69.291	25.239

*Data above 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp° = 30.494 + 2.254\times10^{-3}T - 2.568\times10^{5}T^{-2}$

$H°- H°_{298} = 30.494\times10^{-3}T + 1.127\times10^{-6}T^{2} + 2.568\times10^{2}T^{-1} - 10.053$

Formation equations (kcal/mol):

298.15-600 K: $\Delta Hf° = -117.104 + 8.463\times10^{-3}T - 0.234\times10^{-6}T^{2} + 179.400T^{-1}$

$\Delta Gf° = -117.104 - 8.463\times10^{-3}T\ln T + 0.234\times10^{-6}T^{2} + 89.700T^{-1} + 133.401\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Shchukarev (210). Low-temperature heat capacities and entropy at 298 K from Kiwia (130). High-temperature data estimated.

$MoCl_4(g)$

Molybdenum Tetrachloride (ideal gas)

[Formation: $Mo(c) + 2Cl_2(g) = MoCl_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	23.448	88.869	88.869	0	-92.000	-84.677	62.069
300	23.473	89.014	88.871	.043	-91.998	-84.632	61.654
400	24.412	95.911	89.804	2.443	-91.845	-82.200	44.912
500	24.893	101.416	91.594	4.911	-91.690	-79.805	34.882
600	25.168	105.981	93.623	7.415	-91.549	-77.442	28.208
700	25.339	109.874	95.673	9.941	-91.416	-75.101	23.447
800	25.452	113.266	97.665	12.481	-91.297	-72.781	19.883
900	25.531	116.268	99.568	15.030	-91.187	-70.472	17.113
1000	25.587	118.961	101.374	17.587	-91.088	-68.177	14.900
1100	25.630	121.402	103.086	20.148	-91.005	-65.890	13.091
1200	25.663	123.634	104.707	22.712	-90.939	-63.610	11.585
1300	25.691	125.689	106.243	25.280	-90.890	-61.335	10.311
1400	25.714	127.594	107.701	27.850	-90.859	-59.062	9.220
1500	25.735	129.369	109.087	30.423	-90.847	-56.793	8.275
1600	25.756	131.030	110.407	32.997	-90.855	-54.521	7.447
1700	25.777	132.592	111.666	35.574	-90.883	-52.245	6.717
1800	25.799	134.066	112.870	38.153	-90.934	-49.973	6.067
1900	25.823	135.462	114.023	40.734	-91.010	-47.694	5.486
2000	25.848	136.787	115.129	43.317	-91.115	-45.413	4.962

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 25.622 + 0.142\times10^{-3}T - 1.970\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.622\times10^{-3}T + 0.071\times10^{-6}T^2 + 1.970\times10^{2}T^{-1} - 8.306$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -93.357 + 3.591\times10^{-3}T - 1.290\times10^{-6}T^2 + 119.600T^{-1}$

$\Delta Gf^\circ = -93.357 - 3.591\times10^{-3}T\ln T + 1.290\times10^{-6}T^2 + 59.800T^{-1} + 48.516\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$MoCl_5$(c,l,g)
Molybdenum Pentachloride
[Formation: Mo(c) + 2.5Cl_2(g) = $MoCl_5$(c,l,g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	37.200	57.000	57.000	0	-126.000	-101.231	74.203
300	37.220	57.230	57.000	.069	-125.979	-101.078	73.634
400	40.000	68.320	58.493	3.931	-124.780	-92.953	50.787
467	41.800	74.652	60.369	6.670	-123.869	-87.694	41.039
467	42.000	84.288	60.369	11.170	-119.369	-87.694	41.039
500	42.000	87.156	62.044	12.556	-118.894	-85.472	37.359
537	42.000	90.154	63.878	14.110	-118.369	-83.017	33.786
537	30.660	112.564	63.878	26.144	-106.335	-83.017	33.786
600	30.895	115.985	69.187	28.079	-106.168	-80.300	29.249
700	31.126	120.766	76.222	31.181	-105.898	-76.010	23.731
800	31.280	124.933	82.057	34.301	-105.643	-71.761	19.604
900	31.389	128.624	87.030	37.435	-105.393	-67.539	16.400
1000	31.470	131.935	91.357	40.578	-105.155	-63.349	13.845
1100	31.536	134.938	95.184	43.729	-104.930	-59.178	11.757
1200	31.594	137.685	98.614	46.885	-104.722	-55.029	10.022
1300	31.648	140.216	101.718	50.047	-104.530	-50.896	8.556
1400	31.701	142.563	104.552	53.215	-104.353	-46.775	7.302
1500	31.754	144.752	107.160	56.388	-104.194	-42.669	6.217
1600	31.809	146.803	109.574	59.566	-104.052	-38.571	5.269
1700	31.866	148.733	111.821	62.750	-103.928	-34.478	4.432
1800	31.924	150.556	113.923	65.939	-103.824	-30.399	3.691
1900	31.983	152.284	115.898	69.134	-103.742	-26.320	3.027
2000	32.042	153.926	117.758	72.336	-103.686	-22.247	2.431

*Data except enthalpy of formation at 298 K and temperature of fusion estimated.

Phase changes: 467 K, melting point of $MoCl_5$; ΔH° = 4.500 kcal/mol.
537 K, boiling point of $MoCl_5$; ΔH° = 12.034 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-467 K: $Cp^\circ = 29.079 + 27.246\times10^{-3}T$

$H^\circ - H^\circ_{298} = 29.079\times10^{-3}T + 13.623\times10^{-6}T^2 - 9.881$

467.00-537 K: $Cp^\circ = 42.000$

$H^\circ - H^\circ_{298} = 42.000\times10^{-3}T - 8.444$

537-2000 K: $Cp^\circ = 31.506 + 0.256\times10^{-3}T - 2.837\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 31.506\times10^{-3}T + 0.128\times10^{-6}T^2 + 2.837\times10^{2}T^{-1} + 8.660$

Formation equations (kcal/mol):

298.15-467 K: $\Delta Hf^\circ = -127.497 + 2.635\times10^{-3}T + 12.218\times10^{-6}T^2 - 111.550T^{-1}$

$\Delta Gf^\circ = -127.497 - 2.635\times10^{-3}T\ln T - 12.218\times10^{-6}T^2 - 55.775T^{-1} + 107.378\times10^{-3}T$

467-537 K: $\Delta Hf^\circ = -126.061 + 15.556\times10^{-3}T - 1.405\times10^{-6}T^2 - 111.550T^{-1}$

$\Delta Gf^\circ = -126.061 - 15.556\times10^{-3}T\ln T + 1.405\times10^{-6}T^2 - 55.775T^{-1} + 177.356\times10^{-3}T$

537-2000 K: $\Delta Hf^\circ = -108.956 + 5.062\times10^{-3}T - 1.277\times10^{-6}T^2 + 172.150T^{-1}$

$\Delta Gf^\circ = -108.956 - 5.062\times10^{-3}T\ln T + 1.277\times10^{-6}T^2 + 86.075T^{-1} + 79.116\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K and temperature of fusion.

$MoCl_5(g)$

Molybdenum Pentachloride (ideal gas)

[Formation: $Mo(c) + 2.5Cl_2(g) = MoCl_5(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	28.556	95.043	95.043	0	-107.000	-93.574	68.590
300	28.590	95.220	95.043	.053	-106.995	-93.491	68.107
400	29.868	103.642	96.182	2.984	-106.727	-89.029	48.643
500	30.522	110.384	98.372	6.006	-106.444	-84.636	36.994
600	30.895	115.985	100.853	9.079	-106.168	-80.300	29.249
700	31.126	120.766	103.365	12.181	-105.898	-76.010	23.731
800	31.280	124.933	105.807	15.301	-105.642	-71.761	19.604
900	31.389	128.624	108.141	18.435	-105.393	-67.539	16.400
1000	31.470	131.935	110.357	21.578	-105.155	-63.349	13.845
1100	31.536	134.938	112.457	24.729	-104.930	-59.178	11.757
1200	31.594	137.685	114.448	27.885	-104.722	-55.029	10.022
1300	31.648	140.216	116.334	31.047	-104.530	-50.896	8.556
1400	31.701	142.563	118.124	34.215	-104.353	-46.775	7.302
1500	31.754	144.752	119.827	37.388	-104.194	-42.669	6.217
1600	31.809	146.803	121.449	40.566	-104.052	-38.571	5.269
1700	31.866	148.733	122.998	43.750	-103.928	-34.478	4.432
1800	31.924	150.556	124.479	46.939	-103.824	-30.399	3.691
1900	31.983	152.284	125.898	50.134	-103.742	-26.320	3.027
2000	32.042	153.926	127.258	53.336	-103.686	-22.247	2.431

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 31.440 + 0.292\times10^{-3}T - 2.641\times10^{5}T^{-2}$

$H°- H°_{298} = 31.440\times10^{-3}T + 0.146\times10^{-6}T^{2} + 2.641\times10^{2}T^{-1} - 10.273$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -108.889 + 4.996\times10^{-3}T - 1.259\times10^{-6}T^{2} + 152.550T^{-1}$

$\Delta Gf° = -108.889 - 4.996\times10^{-3}T\ln T + 1.259\times10^{-6}T^{2} + 76.275T^{-1} + 78.597\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$MoCl_6(g)$
Molybdenum Hexachloride (ideal gas)
[Formation: $Mo(c) + 3Cl_2(g) = MoCl_6(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	34.446	100.272	100.272	0	-105.000	-85.189	62.444
300	34.482	100.485	100.272	.064	-104.992	-85.066	61.970
400	35.815	110.612	101.645	3.587	-104.546	-78.492	42.885
500	36.482	118.683	104.273	7.205	-104.094	-72.028	31.483
600	36.859	125.371	107.248	10.874	-103.657	-65.657	23.915
700	37.092	131.072	110.255	14.572	-103.230	-59.358	18.532
800	37.244	136.035	113.173	18.290	-102.819	-53.120	14.511
900	37.350	140.428	115.961	22.020	-102.418	-46.929	11.396
1000	37.427	144.368	118.609	25.759	-102.031	-40.789	8.914
1100	37.483	147.938	121.116	29.504	-101.661	-34.683	6.891
1200	37.526	151.201	123.489	33.255	-101.308	-28.608	5.210
1300	37.560	154.206	125.738	37.009	-100.975	-22.564	3.793
1400	37.587	156.991	127.872	40.767	-100.660	-16.544	2.583
1500	37.609	159.585	129.900	44.527	-100.367	-10.547	1.537
1600	37.626	162.013	131.833	48.288	-100.096	-4.568	.624
1700	37.641	164.294	133.675	52.052	-99.846	1.401	-.180
1800	37.654	166.446	135.437	55.817	-99.622	7.347	-.892
1900	37.664	168.482	137.123	59.582	-99.426	13.288	-1.528
2000	37.673	170.414	138.740	63.349	-99.262	19.214	-2.100

*Data estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 37.552 + 0.128\times10^{-3}T - 2.795\times10^{5}T^{-2}$

$H°- H°_{298} = 37.552\times10^{-3}T + 0.064\times10^{-6}T^{2} + 2.795\times10^{2}T^{-1} - 12.139$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -107.321 + 6.694\times10^{-3}T - 1.385\times10^{-6}T^{2} + 133.800T^{-1}$

$\Delta Gf° = -107.321 - 6.694\times10^{-3}T\ln T + 1.385\times10^{-6}T^{2} + 66.900T^{-1} + 111.208\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

MoF(g)

Molybdenum Monofluoride (ideal gas)

[Formation: $Mo(c) + 0.5F_2(g) = MoF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	7.809	58.865	58.865	0	67.600	59.313	-43.477
300	7.817	58.913	58.866	.014	67.596	59.261	-43.171
400	8.188	61.216	59.176	.816	67.426	56.509	-30.875
500	8.426	63.071	59.775	1.648	67.250	53.801	-23.516
600	8.580	64.622	60.459	2.498	67.060	51.127	-18.623
700	8.684	65.953	61.150	3.362	66.862	48.489	-15.139
800	8.758	67.117	61.824	4.234	66.655	45.878	-12.533
900	8.813	68.152	62.471	5.113	66.439	43.294	-10.513
1000	8.856	69.083	63.087	5.996	66.212	40.732	-8.902
1100	8.890	69.929	63.671	6.884	65.973	38.197	-7.589
1200	8.918	70.704	64.226	7.774	65.719	35.683	-6.499
1300	8.943	71.418	64.751	8.667	65.450	33.192	-5.580
1400	8.965	72.082	65.251	9.563	65.165	30.721	-4.796
1500	8.988	72.701	65.728	10.460	64.861	28.270	-4.119
1600	9.012	73.282	66.182	11.360	64.542	25.842	-3.530
1700	9.040	73.829	66.615	12.263	64.204	23.434	-3.013
1800	9.074	74.347	67.031	13.169	63.846	21.046	-2.555
1900	9.117	74.839	67.430	14.078	63.466	18.677	-2.148
2000	9.169	75.308	67.812	14.992	63.063	16.330	-1.784

*Data estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.605 + 0.294\times10^{-3}T - 0.785\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.605\times10^{-3}T + 0.147\times10^{-6}T^2 + 0.785\times10^{2}T^{-1} - 2.842$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = 67.414 - 0.026\times10^{-3}T - 1.125\times10^{-6}T^2 + 87.450T^{-1}$

$\Delta Gf^\circ = 67.414 + 0.026\times10^{-3}T\ln T + 1.125\times10^{-6}T^2 + 43.725T^{-1} - 28.147\times10^{-3}T$

Source: Data are estimations from JANAF (62).

$MoF_2(g)$
Molybdenum Difluoride (ideal gas)
[Formation: $Mo(c) + F_2(g) = MoF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	13.676	64.967	64.967	0	-38.900	-41.784	30.628
300	13.691	65.052	64.969	.025	-38.900	-41.803	30.453
400	14.210	69.072	65.512	1.424	-38.857	-42.777	23.372
500	14.450	72.272	66.556	2.858	-38.834	-43.760	19.127
600	14.580	74.919	67.736	4.310	-38.837	-44.746	16.298
700	14.660	77.173	68.926	5.773	-38.859	-45.727	14.277
800	14.712	79.134	70.082	7.242	-38.901	-46.707	12.759
900	14.749	80.869	71.186	8.715	-38.958	-47.678	11.578
1000	14.776	82.425	72.234	10.191	-39.032	-48.646	10.631
1100	14.797	83.834	73.225	11.670	-39.123	-49.602	9.855
1200	14.813	85.122	74.164	13.150	-39.232	-50.549	9.206
1300	14.825	86.308	75.053	14.632	-39.360	-51.486	8.656
1400	14.835	87.407	75.896	16.115	-39.508	-52.415	8.182
1500	14.843	88.431	76.698	17.599	-39.676	-53.332	7.770
1600	14.850	89.389	77.462	19.084	-39.863	-54.234	7.408
1700	14.856	90.290	78.191	20.569	-40.073	-55.127	7.087
1800	14.861	91.139	78.886	22.055	-40.307	-56.005	6.800
1900	14.865	91.943	79.553	23.541	-40.567	-56.871	6.542
2000	14.869	92.705	80.191	25.028	-40.855	-57.721	6.307

*Data estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 14.868 + 0.014\times10^{-3}T - 1.063\times10^{5}T^{-2}$

$H°- H°_{298} = 14.868\times10^{-3}T + 0.007\times10^{-6}T^{2} + 1.063\times10^{2}T^{-1} - 4.790$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -39.589 + 1.983\times10^{-3}T - 1.352\times10^{-6}T^{2} + 65.000T^{-1}$

$\Delta Gf° = -39.589 - 1.983\times10^{-3}T\ln T + 1.352\times10^{-6}T^{2} + 32.500T^{-1} + 3.167\times10^{-3}T$

Source: Data are estimations from JANAF (62).

$MoF_3(g)$

Molybdenum Trifluoride (ideal gas)

[Formation: $Mo(c) + 1.5F_2(g) = MoF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	16.035	70.712	70.712	0	-145.100	-142.476	104.436
300	16.068	70.811	70.712	.030	-145.102	-142.459	103.780
400	17.408	75.635	71.360	1.710	-145.163	-141.567	77.348
500	18.185	79.610	72.624	3.493	-145.193	-140.664	61.483
600	18.677	82.973	74.076	5.338	-145.218	-139.757	50.906
700	19.025	85.879	75.560	7.223	-145.242	-138.845	43.349
800	19.297	88.438	77.013	9.140	-145.267	-137.931	37.680
900	19.525	90.724	78.412	11.081	-145.291	-137.011	33.270
1000	19.725	92.792	79.748	13.044	-145.318	-136.091	29.742
1100	19.900	94.680	81.021	15.025	-145.350	-135.166	26.855
1200	20.054	96.418	82.232	17.023	-145.387	-134.238	24.448
1300	20.189	98.029	83.386	19.036	-145.431	-133.306	22.410
1400	20.307	99.530	84.486	21.061	-145.487	-132.373	20.664
1500	20.409	100.934	85.536	23.097	-145.555	-131.434	19.150
1600	20.499	102.254	86.540	25.142	-145.635	-130.489	17.824
1700	20.579	103.500	87.502	27.196	-145.730	-129.540	16.653
1800	20.651	104.678	88.424	29.257	-145.845	-128.584	15.612
1900	20.719	105.796	89.309	31.326	-145.978	-127.620	14.679
2000	20.784	106.861	90.160	33.401	-146.137	-126.652	13.840

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 18.632 + 1.280\times10^{-3}T - 2.647\times10^{5}T^{-2}$

$H°- H°_{298} = 18.632\times10^{-3}T + 0.640\times10^{-6}T^{2} + 2.647\times10^{2}T^{-1} - 6.500$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -146.054 + 1.493\times10^{-3}T - 0.806\times10^{-6}T^{2} + 173.150T^{-1}$

$\Delta Gf° = -146.054 - 1.493\times10^{-3}T\ln T + 0.806\times10^{-6}T^{2} + 86.575T^{-1} + 19.295\times10^{-3}T$

Source: Data from JANAF (62). All are estimations except enthalpy of formation at 298 K.

$MoF_4(g)$

Molybdenum Tetrafluoride (ideal gas)

[Formation: $Mo(c) + 2F_2(g) = MoF_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	20.371	78.592	78.592	0	-226.500	-219.003	160.532
300	20.411	78.718	78.592	.038	-226.501	-218.957	159.508
400	22.134	84.845	79.415	2.172	-226.492	-216.441	118.256
500	23.217	89.910	81.024	4.443	-226.436	-213.934	93.509
600	23.909	94.208	82.871	6.802	-226.362	-211.441	77.016
700	24.368	97.931	84.764	9.217	-226.280	-208.961	65.240
800	24.684	101.207	86.618	11.671	-226.199	-206.493	56.411
900	24.910	104.128	88.405	14.151	-226.120	-204.033	49.545
1000	25.077	106.761	90.110	16.651	-226.050	-201.585	44.056
1100	25.202	109.158	91.735	19.165	-225.992	-199.141	39.565
1200	25.300	111.355	93.279	21.691	-225.946	-196.701	35.824
1300	25.376	113.383	94.749	24.224	-225.918	-194.264	32.658
1400	25.438	115.266	96.148	26.765	-225.908	-191.832	29.946
1500	25.488	117.023	97.482	29.312	-225.916	-189.399	27.595
1600	25.530	118.669	98.755	31.863	-225.943	-186.961	25.537
1700	25.566	120.218	99.972	34.418	-225.991	-184.521	23.722
1800	25.598	121.680	101.138	36.976	-226.065	-182.080	22.107
1900	25.627	123.065	102.256	39.537	-226.163	-179.634	20.662
2000	25.655	124.380	103.329	42.101	-226.291	-177.183	19.361

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 24.412 + 0.878\times10^{-3}T - 3.825\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 24.412\times10^{-3}T + 0.439\times10^{-6}T^2 + 3.825\times10^{2}T^{-1} - 8.600$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -228.110 + 3.019\times10^{-3}T - 1.094\times10^{-6}T^2 + 240.700T^{-1}$

$\Delta Gf^\circ = -228.110 - 3.019\times10^{-3}T\ln T + 1.094\times10^{-6}T^2 + 120.350T^{-1} + 46.066\times10^{-3}T$

Source: Data from JANAF (62). All are estimations except enthalpy of formation at 298 K.

$MoF_5(g)$

Molybdenum Pentafluoride (ideal gas)

[Formation: $Mo(c) + 2.5F_2(g) = MoF_5(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	24.561	83.065	83.065	0	-296.700	-283.315	207.673
300	24.626	83.217	83.067	.045	-296.701	-283.234	206.333
400	27.403	90.714	84.069	2.658	-296.598	-278.754	152.302
500	29.078	97.025	86.047	5.489	-296.383	-274.316	119.902
600	30.073	102.422	88.337	8.451	-296.122	-269.928	98.320
700	30.670	107.107	90.691	11.491	-295.839	-265.583	82.918
800	31.038	111.228	93.006	14.578	-295.556	-261.282	71.378
900	31.271	114.898	95.238	17.694	-295.276	-257.012	62.410
1000	31.424	118.201	97.372	20.829	-295.011	-252.779	55.244
1100	31.529	121.202	99.405	23.977	-294.762	-248.566	49.385
1200	31.605	123.949	101.337	27.134	-294.531	-244.377	44.507
1300	31.663	126.481	103.175	30.298	-294.319	-240.204	40.381
1400	31.710	128.829	104.925	33.466	-294.132	-236.052	36.849
1500	31.751	131.018	106.592	36.639	-293.966	-231.910	33.789
1600	31.788	133.068	108.183	39.816	-293.820	-227.775	31.112
1700	31.823	134.997	109.705	42.997	-293.696	-223.650	28.752
1800	31.856	136.817	111.161	46.181	-293.600	-219.533	26.655
1900	31.888	138.540	112.557	49.368	-293.528	-215.419	24.779
2000	31.919	140.176	113.896	52.559	-293.488	-211.309	23.091

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 31.515 + 0.376\times10^{-3}T - 6.281\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 31.515\times10^{-3}T + 0.188\times10^{-6}T^2 + 6.281\times10^{2}T^{-1} - 11.520$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -299.785 + 5.868\times10^{-3}T - 1.432\times10^{-6}T^2 + 436.050T^{-1}$

$\Delta Gf^\circ = -299.785 - 5.868\times10^{-3}T\ln T + 1.432\times10^{-6}T^2 + 218.025T^{-1} + 85.793\times10^{-3}T$

Source: Data from JANAF (62) who estimated some molecular constants.

$MoF_6(g)$

Molybdenum Hexafluoride (ideal gas)

[Formation: $Mo(c) + 3F_2(g) = MoF_6(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	28.747	83.796	83.796	0	-372.290	-351.902	257.948
300	28.818	83.974	83.797	.053	-372.290	-351.776	256.266
400	31.806	92.710	84.967	3.097	-372.140	-344.955	188.472
500	33.601	100.017	87.267	6.375	-371.881	-338.186	147.819
600	34.722	106.250	89.925	9.795	-371.576	-331.477	120.739
700	35.456	111.661	92.651	13.307	-371.245	-324.818	101.412
800	35.958	116.430	95.331	16.879	-370.908	-318.211	86.930
900	36.315	120.687	97.917	20.493	-370.566	-311.642	75.676
1000	36.576	124.528	100.389	24.139	-370.230	-305.117	66.682
1100	36.774	128.023	102.744	27.807	-369.904	-298.618	59.329
1200	36.926	131.230	104.987	31.492	-369.590	-292.153	53.208
1300	37.045	134.190	107.120	35.191	-369.291	-285.709	48.031
1400	37.141	136.939	109.153	38.900	-369.013	-279.294	43.599
1500	37.219	139.505	111.093	42.618	-368.753	-272.897	39.761
1600	37.283	141.909	112.945	46.343	-368.512	-266.512	36.403
1700	37.336	144.171	114.716	50.074	-368.292	-260.141	33.443
1800	37.381	146.306	116.412	53.810	-368.100	-253.786	30.813
1900	37.419	148.328	118.039	57.550	-367.932	-247.438	28.461
2000	37.451	150.248	119.601	61.294	-367.797	-241.101	26.346

Phase changes: 290.76 K, melting point of MoF_6; ΔH° = 1.034 kcal/mol.
307.04 K, boiling point to real gas; ΔH° = 6.574 kcal/mol.
308.0 K, boiling point to ideal gas; ΔH° = 6.511 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 35.749 + 1.240\times10^{-3}T - 6.553\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 35.749\times10^{-3}T + 0.620\times10^{-6}T^2 + 6.553\times10^{2}T^{-1} - 12.912$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -375.322 + 5.848\times10^{-3}T - 1.087\times10^{-6}T^2 + 413.000T^{-1}$

$\Delta Gf^\circ = -375.322 - 5.848\times10^{-3}T\ln T + 1.087\times10^{-6}T^2 + 206.500T^{-1} + 109.226\times10^{-3}T$

Source: Data from JANAF (61).

MoI(g)

Molybdenum Monoiodide (ideal gas)

[Formation: $Mo(c) + 0.5I_2(c,l,g) = MoI(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	8.834	66.650	66.650	0	119.200	105.509	-77.339
300	8.836	66.705	66.652	.016	119.193	105.423	-76.800
386.8	8.901	68.960	66.927	.786	118.851	101.482	-57.339
386.8	8.901	68.960	66.927	.786	116.997	101.482	-57.339
400	8.911	69.259	66.999	.904	116.908	100.954	-55.158
458.4	8.936	70.475	67.364	1.426	116.515	98.655	-47.035
458.4	8.936	70.475	67.364	1.426	111.505	98.655	-47.035
500	8.954	71.252	67.656	1.798	111.436	97.492	-42.613
600	8.983	72.887	68.397	2.694	111.258	94.718	-34.501
700	9.006	74.274	69.140	3.594	111.072	91.977	-28.716
800	9.026	75.478	69.858	4.496	110.874	89.263	-24.385
900	9.043	76.542	70.543	5.399	110.666	86.573	-21.023
1000	9.060	77.495	71.191	6.304	110.449	83.907	-18.338
1100	9.075	78.360	71.805	7.211	110.218	81.264	-16.145
1200	9.090	79.150	72.384	8.119	109.974	78.643	-14.323
1300	9.106	79.878	72.933	9.029	109.715	76.043	-12.784
1400	9.123	80.554	73.454	9.940	109.438	73.463	-11.468
1500	9.142	81.184	73.948	10.854	109.147	70.902	-10.330
1600	9.164	81.774	74.418	11.769	108.839	68.365	-9.338
1700	9.191	82.331	74.868	12.687	108.512	65.845	-8.465
1800	9.225	82.857	75.298	13.607	108.165	63.345	-7.691
1900	9.269	83.357	75.709	14.532	107.798	60.864	-7.001
2000	9.323	83.834	76.104	15.461	107.409	58.403	-6.382

*Data estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.922 + 0.156\times10^{-3}T - 0.119\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.922\times10^{-3}T + 0.078\times10^{-6}T^2 + 0.119\times10^{2}T^{-1} - 2.707$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = 119.691 - 1.894\times10^{-3}T - 1.853\times10^{-6}T^2 + 71.100T^{-1}$

$\Delta Gf^\circ = 119.691 + 1.894\times10^{-3}T\ln T + 1.853\times10^{-6}T^2 + 35.550T^{-1} - 59.308\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = 118.963 - 5.096\times10^{-3}T - 1.107\times10^{-6}T^2 + 71.100T^{-1}$

$\Delta Gf^\circ = 118.963 + 5.096\times10^{-3}T\ln T + 1.107\times10^{-6}T^2 + 35.550T^{-1} - 76.216\times10^{-3}T$

458.4-2000 K: $\Delta Hf^\circ = 111.607 + 0.074\times10^{-3}T - 1.141\times10^{-6}T^2 + 63.450T^{-1}$

$\Delta Gf^\circ = 111.607 - 0.074\times10^{-3}T\ln T + 1.141\times10^{-6}T^2 + 31.725T^{-1} - 28.484\times10^{-3}T$

Source: Data from JANAF (61). All are estimations.

$MoI_2(c)$
Molybdenum Diiodide
[Formation: $Mo(c) + I_2(c,l,g) = MoI_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	19.767	35.770	35.770	0	-24.840	-25.186	18.462
300	19.773	35.892	35.770	.037	-24.838	-25.188	18.349
386.8	20.032	40.948	36.387	1.764	-24.827	-25.295	14.292
386.8	20.032	40.948	36.387	1.764	-28.536	-25.295	14.292
400	20.071	41.621	36.549	2.029	-28.605	-25.183	13.759
458.4	20.245	44.368	37.374	3.206	-28.905	-24.660	11.757
458.4	20.245	44.368	37.374	3.206	-38.926	-24.660	11.757
500	20.369	46.132	38.030	4.051	-38.708	-23.373	10.216
600	20.667	49.872	39.700	6.103	-38.178	-20.357	7.415
700	20.965	53.080	41.389	8.184	-37.633	-17.430	5.442
800	21.263	55.899	43.029	10.296	-37.071	-14.581	3.983
900	21.561	58.421	44.602	12.437	-36.493	-11.805	2.867
1000	21.859	60.708	46.100	14.608	-35.897	-9.094	1.987
1100	22.157	62.806	47.525	16.809	-35.287	-6.444	1.280
1200	22.455	64.746	48.880	19.039	-34.664	-3.848	.701
1300	22.753	66.555	50.170	21.300	-34.027	-1.305	.219

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
1305 K, pressure of decomposition products, $I_2(g)$ and $I(g)$, = 1 atm. Decomposition begins near 1060 K.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $Cp^\circ = 18.888 + 2.970\times10^{-3}T - 0.006\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 18.888\times10^{-3}T + 1.485\times10^{-6}T^2 + 0.006\times10^{2}T^{-1} - 5.765$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -25.422 + 1.634\times10^{-3}T - 1.192\times10^{-6}T^2 + 59.800T^{-1}$

$\Delta Gf^\circ = -25.422 - 1.634\times10^{-3}T\ln T + 1.192\times10^{-6}T^2 + 29.900T^{-1} + 9.407\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -26.877 - 4.770\times10^{-3}T + 0.300\times10^{-6}T^2 + 59.800T^{-1}$

$\Delta Gf^\circ = -26.877 + 4.770\times10^{-3}T\ln T - 0.300\times10^{-6}T^2 + 29.900T^{-1} - 24.408\times10^{-3}T$

458.4-1300 K: $\Delta Hf^\circ = -41.590 + 5.570\times10^{-3}T + 0.232\times10^{-6}T^2 + 44.500T^{-1}$

$\Delta Gf^\circ = -41.590 - 5.570\times10^{-3}T\ln T - 0.232\times10^{-6}T^2 + 22.250T^{-1} + 71.055\times10^{-3}T$

Source: Data from JANAF (61). All are estimations except enthalpy of formation at 298 K.

$MoI_2(g)$

Molybdenum Diiodide (ideal gas)

[Formation: $Mo(c) + I_2(c,l,g) = MoI_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	16.902	81.066	81.066	0	61.600	47.749	-35.000
300	16.906	81.171	81.068	.031	61.596	47.662	-34.721
386.8	17.014	85.484	81.595	1.504	61.353	43.659	-24.668
386.8	17.014	85.484	81.595	1.504	57.644	43.659	-24.668
400	17.030	86.055	81.732	1.729	57.535	43.183	-23.594
458.4	17.015	88.377	82.434	2.724	57.053	41.124	-19.606
458.4	17.015	88.377	82.434	2.724	47.032	41.124	-19.606
500	17.004	89.855	82.991	3.432	47.113	40.586	-17.740
600	16.874	92.945	84.400	5.127	47.286	39.263	-14.301
700	16.689	95.533	85.812	6.805	47.428	37.914	-11.837
800	16.490	97.748	87.168	8.464	47.537	36.548	-9.984
900	16.300	99.679	88.452	10.104	47.614	35.170	-8.540
1000	16.128	101.387	89.662	11.725	47.660	33.784	-7.383
1100	15.977	102.917	90.799	13.330	47.674	32.395	-6.436
1200	15.847	104.302	91.868	14.921	47.658	31.007	-5.647
1300	15.737	105.566	92.874	16.500	47.613	29.621	-4.980
1400	15.643	106.728	93.822	18.069	47.539	28.241	-4.409
1500	15.563	107.805	94.719	19.629	47.437	26.863	-3.914
1600	15.497	108.807	95.568	21.182	47.310	25.499	-3.483
1700	15.442	109.745	96.375	22.729	47.154	24.139	-3.103
1800	15.397	110.626	97.142	24.271	46.971	22.792	-2.767
1900	15.361	111.458	97.875	25.808	46.756	21.452	-2.467
2000	15.334	112.245	98.574	27.343	46.513	20.127	-2.199

*Data estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 17.701 - 1.392\times10^{-3}T - 0.341\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 17.701\times10^{-3}T - 0.696\times10^{-6}T^2 + 0.341\times10^{2}T^{-1} - 5.330$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = 61.454 + 0.447\times10^{-3}T - 3.373\times10^{-6}T^2 + 93.300T^{-1}$

$\Delta Gf^\circ = 61.454 - 0.447\times10^{-3}T\ln T + 3.373\times10^{-6}T^2 + 46.650T^{-1} - 44.951\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = 59.998 - 5.957\times10^{-3}T - 1.881\times10^{-6}T^2 + 93.300T^{-1}$

$\Delta Gf^\circ = 59.998 + 5.957\times10^{-3}T\ln T + 1.881\times10^{-6}T^2 + 46.650T^{-1} - 78.766\times10^{-3}T$

458.4-2000 K: $\Delta Hf^\circ = 45.285 + 4.383\times10^{-3}T - 1.949\times10^{-6}T^2 + 78.000T^{-1}$

$\Delta Gf^\circ = 45.285 - 4.383\times10^{-3}T\ln T + 1.949\times10^{-6}T^2 + 39.000T^{-1} + 16.697\times10^{-3}T$

Source: Data from JANAF (61). All are estimations.

$MoI_3(g)$

Molybdenum Triiodide (ideal gas)

[Formation: $Mo(c) + 1.5I_2(c,l,g) = MoI_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15*	19.482	96.420	96.420	0	43.700	29.409	-21.557
300	19.487	96.541	96.421	.036	43.689	29.320	-21.359
386.8	19.631	101.514	97.029	1.735	43.067	25.238	-14.260
386.8	19.631	101.514	97.029	1.735	37.504	25.238	-14.260
400	19.653	102.173	97.188	1.994	37.302	24.823	-13.563
458.4	19.703	104.855	97.997	3.144	36.412	23.068	-10.998
458.4	19.703	104.855	97.997	3.144	21.380	23.068	-10.998
500	19.738	106.568	98.640	3.964	21.388	23.223	-10.151
600	19.804	110.172	100.270	5.941	21.395	23.587	-8.592
700	19.876	113.231	101.910	7.925	21.393	23.953	-7.478
800	19.960	115.890	103.494	9.917	21.385	24.321	-6.644
900	20.056	118.246	105.005	11.917	21.369	24.687	-5.995
1000	20.158	120.365	106.437	13.928	21.353	25.057	-5.476
1100	20.261	122.291	107.792	15.949	21.329	25.428	-5.052
1200	20.359	124.058	109.075	17.980	21.299	25.803	-4.699
1300	20.450	125.691	110.290	20.021	21.262	26.181	-4.401
1400	20.532	127.210	111.446	22.070	21.212	26.561	-4.146
1500	20.606	128.629	112.544	24.127	21.150	26.942	-3.925
1600	20.672	129.961	113.592	26.191	21.077	27.335	-3.734
1700	20.732	131.216	114.592	28.261	20.986	27.727	-3.565
1800	20.789	132.403	115.549	30.337	20.879	28.126	-3.415
1900	20.843	133.528	116.465	32.419	20.749	28.533	-3.282
2000	20.895	134.598	117.345	34.506	20.598	28.948	-3.163

*Data estimated.

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.352 + 0.824\times10^{-3}T - 0.103\times10^{5}T^{-2}$

$H°- H°_{298} = 19.352\times10^{-3}T + 0.412\times10^{-6}T^{2} + 0.103\times10^{2}T^{-1} - 5.841$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = 45.029 - 4.340\times10^{-3}T - 3.011\times10^{-6}T^{2} + 69.500T^{-1}$

$\Delta Gf° = 45.029 + 4.340\times10^{-3}T\ln T + 3.011\times10^{-6}T^{2} + 34.750T^{-1} - 78.408\times10^{-3}T$

386.8-458.4 K: $\Delta Hf° = 42.846 - 13.947\times10^{-3}T - 0.773\times10^{-6}T^{2} + 69.500T^{-1}$

$\Delta Gf° = 42.846 + 13.947\times10^{-3}T\ln T + 0.773\times10^{-6}T^{2} + 34.750T^{-1} - 129.131\times10^{-3}T$

458.4-2000 K: $\Delta Hf° = 20.776 + 1.564\times10^{-3}T - 0.875\times10^{-6}T^{2} + 46.550T^{-1}$

$\Delta Gf° = 20.776 - 1.564\times10^{-3}T\ln T + 0.875\times10^{-6}T^{2} + 23.275T^{-1} + 14.063\times10^{-3}T$

Source: Data from JANAF (61). All are estimations.

$MoI_4(g)$

Molybdenum Tetraiodide (ideal gas)

[Formation: $Mo(c) + 2I_2(c,l,g) = MoI_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	25.064	108.198	108.198	0	29.800	16.135	-11.827
300	25.073	108.353	108.200	.046	29.787	16.050	-11.692
386.8	25.352	114.766	108.982	2.237	29.054	12.165	-6.873
386.8	25.352	114.766	108.982	2.237	21.636	12.165	-6.873
400	25.395	115.617	109.187	2.572	21.382	11.846	-6.472
458.4	25.486	119.085	110.232	4.058	20.266	10.537	-5.023
458.4	25.486	119.085	110.232	4.058	.224	10.537	-5.023
500	25.550	121.302	111.062	5.120	.287	11.473	-5.015
600	25.635	125.969	113.169	7.680	.428	13.695	-4.988
700	25.687	129.925	115.288	10.246	.559	15.896	-4.963
800	25.721	133.357	117.336	12.817	.679	18.081	-4.939
900	25.745	136.388	119.288	15.390	.785	20.247	-4.917
1000	25.761	139.101	121.136	17.965	.880	22.405	-4.897
1100	25.774	141.557	122.882	20.542	.959	24.553	-4.878
1200	25.783	143.800	124.533	23.120	1.021	26.696	-4.862
1300	25.791	145.864	126.096	25.699	1.067	28.835	-4.848
1400	25.797	147.776	127.577	28.278	1.091	30.970	-4.835
1500	25.802	149.556	128.984	30.858	1.096	33.100	-4.823
1600	25.807	151.221	130.322	33.439	1.083	35.240	-4.813
1700	25.812	152.786	131.598	36.020	1.045	37.374	-4.805
1800	25.818	154.262	132.817	38.601	.984	39.511	-4.797
1900	25.825	155.658	133.983	41.183	.895	41.654	-4.791
2000	25.834	156.983	135.100	43.766	.780	43.802	-4.786

*Data estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 25.812 + 0.014\times10^{-3}T - 0.669\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.812\times10^{-3}T + 0.007\times10^{-6}T^2 + 0.669\times10^{2}T^{-1} - 7.921$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = 31.035 - 4.319\times10^{-3}T - 4.162\times10^{-6}T^2 + 126.100T^{-1}$

$\Delta Gf^\circ = 31.035 + 4.319\times10^{-3}T\ln T + 4.162\times10^{-6}T^2 + 63.050T^{-1} - 76.531\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = 28.124 - 17.127\times10^{-3}T - 1.178\times10^{-6}T^2 + 126.100T^{-1}$

$\Delta Gf^\circ = 28.124 + 17.127\times10^{-3}T\ln T + 1.178\times10^{-6}T^2 + 63.050T^{-1} - 144.162\times10^{-3}T$

458.4-2000 K: $\Delta Hf^\circ = -1.302 + 3.553\times10^{-3}T - 1.314\times10^{-6}T^2 + 95.500T^{-1}$

$\Delta Gf^\circ = -1.302 - 3.553\times10^{-3}T\ln T + 1.314\times10^{-6}T^2 + 47.750T^{-1} + 46.764\times10^{-3}T$

Source: Data from JANAF (61). All are estimations.

NBr(g)

Nitrogen Monobromide (ideal gas)

[Formation: $0.5N_2(g) + 0.5Br_2(l,g) = NBr(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔH_f°	ΔG_f°	
298.15	7.819	56.256	56.256	0	71.900	67.374	-49.386
300	7.828	56.305	56.258	.014	71.891	67.345	-49.060
332.6	7.948	57.119	56.303	.271	71.741	66.859	-43.932
332.6	7.948	57.119	56.303	.271	68.208	66.859	-43.932
400	8.196	58.611	56.569	.817	68.225	66.583	-36.379
500	8.430	60.467	57.169	1.649	68.264	66.168	-28.922
600	8.581	62.018	57.851	2.500	68.314	65.744	-23.947
700	8.683	63.349	58.543	3.364	68.368	65.312	-20.391
800	8.755	64.514	59.219	4.236	68.422	64.872	-17.722
900	8.808	65.548	59.866	5.114	68.470	64.425	-15.644
1000	8.849	66.478	60.481	5.997	68.516	63.973	-13.981
1100	8.881	67.323	61.065	6.884	68.558	63.517	-12.620
1200	8.907	68.097	61.619	7.773	68.596	63.057	-11.484
1300	8.929	68.811	62.146	8.665	68.630	62.594	-10.523
1400	8.948	69.473	62.645	9.559	68.660	62.130	-9.699
1500	8.964	70.091	63.122	10.454	68.687	61.661	-8.984
1600	8.979	70.670	63.575	11.352	68.712	61.193	-8.358
1700	8.992	71.215	64.009	12.250	68.734	60.721	-7.806
1800	9.004	71.729	64.423	13.150	68.754	60.250	-7.315
1900	9.015	72.216	64.821	14.051	68.773	59.778	-6.876
2000	9.026	72.679	65.202	14.953	68.789	59.303	-6.480

Phase change: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 8.652 + 0.242\times10^{-3}T - 0.805\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.652\times10^{-3}T + 0.121\times10^{-6}T^2 + 0.805\times10^{2}T^{-1} - 2.860$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta H_f^\circ = 72.717 - 3.652\times10^{-3}T - 0.124\times10^{-6}T^2 + 84.450T^{-1}$

$\Delta G_f^\circ = 72.717 + 3.652\times10^{-3}T\ln T + 0.124\times10^{-6}T^2 + 42.225T^{-1} - 39.240\times10^{-3}T$

332.6-2000 K: $\Delta H_f^\circ = 67.716 + 0.929\times10^{-3}T - 0.201\times10^{-6}T^2 + 68.750T^{-1}$

$\Delta G_f^\circ = 67.716 - 0.929\times10^{-3}T\ln T + 0.201\times10^{-6}T^2 + 34.375T^{-1} + 2.438\times10^{-3}T$

Source: Data from JANAF (60).

NF(g)

Nitrogen Monofluoride (ideal gas)

[Formation: $0.5N_2(g) + 0.5F_2(g) = NF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	7.253	51.427	51.427	0	59.500	58.212	-42.670
300	7.259	51.472	51.429	.013	59.500	58.203	-42.400
400	7.604	53.607	51.717	.756	59.510	57.770	-31.564
500	7.913	55.339	52.273	1.533	59.533	57.333	-25.060
600	8.156	56.804	52.909	2.337	59.566	56.890	-20.722
700	8.340	58.075	53.558	3.162	59.603	56.442	-17.622
800	8.480	59.199	54.195	4.003	59.641	55.986	-15.295
900	8.588	60.204	54.807	4.857	59.681	55.528	-13.484
1000	8.674	61.113	55.393	5.720	59.716	55.065	-12.034
1100	8.743	61.943	55.951	6.591	59.750	54.598	-10.848
1200	8.799	62.707	56.484	7.468	59.782	54.127	-9.858
1300	8.846	63.413	56.989	8.351	59.811	53.657	-9.020
1400	8.887	64.070	57.472	9.237	59.837	53.181	-8.302
1500	8.922	64.684	57.932	10.128	59.862	52.706	-7.679
1600	8.953	65.261	58.372	11.022	59.885	52.227	-7.134
1700	8.981	65.805	58.794	11.918	59.905	51.747	-6.652
1800	9.006	66.319	59.198	12.818	59.925	51.268	-6.225
1900	9.029	66.806	59.585	13.719	59.944	50.786	-5.842
2000	9.050	67.270	59.958	14.623	59.960	50.303	-5.497

*Data estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 7.952 + 0.698\times10^{-3}T - 0.807\times10^{5}T^{-2}$

$H°- H°_{298} = 7.952\times10^{-3}T + 0.349\times10^{-6}T^{2} + 0.807\times10^{2}T^{-1} - 2.673$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 59.256 + 0.439\times10^{-3}T - 0.033\times10^{-6}T^{2} + 34.400T^{-1}$

$\Delta Gf° = 59.256 - 0.439\times10^{-3}T\ln T + 0.033\times10^{-6}T^{2} + 17.200T^{-1} - 1.203\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

$NF_2(g)$

Nitrogen Difluoride (ideal gas)

[Formation: $0.5N_2(g) + F_2(g) = NF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	$Cp°$	$S°$	$-(G°- H°_{298})/T$	$H°- H°_{298}$	$\Delta Hf°$	$\Delta Gf°$	
298.15	9.801	59.715	59.715	0	10.100	13.562	-9.941
300	9.822	59.775	59.715	.018	10.097	13.584	-9.896
400	10.851	62.748	60.113	1.054	10.016	14.760	-8.065
500	11.617	65.256	60.898	2.179	9.986	15.951	-6.972
600	12.159	67.425	61.808	3.370	9.990	17.144	-6.244
700	12.544	69.330	62.750	4.606	10.015	18.334	-5.724
800	12.820	71.024	63.680	5.875	10.050	19.520	-5.332
900	13.024	72.546	64.582	7.168	10.093	20.703	-5.027
1000	13.177	73.927	65.449	8.478	10.135	21.877	-4.781
1100	13.295	75.189	66.278	9.802	10.179	23.050	-4.579
1200	13.387	76.350	67.070	11.136	10.222	24.217	-4.410
1300	13.460	77.424	67.825	12.479	10.265	25.384	-4.267
1400	13.519	78.424	68.547	13.828	10.303	26.544	-4.144
1500	13.568	79.358	69.237	15.182	10.340	27.703	-4.036
1600	13.608	80.235	69.897	16.541	10.375	28.859	-3.942
1700	13.641	81.061	70.529	17.904	10.408	30.015	-3.859
1800	13.670	81.842	71.137	19.269	10.437	31.166	-3.784
1900	13.694	82.581	71.719	20.637	10.465	32.318	-3.717
2000	13.714	83.284	72.280	22.008	10.491	33.468	-3.657

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 12.162 + 1.060\times10^{-3}T - 2.380\times10^{5}T^{-2}$

$H°- H°_{298} = 12.162\times10^{-3}T + 0.530\times10^{-6}T^{2} + 2.380\times10^{2}T^{-1} - 4.471$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = 9.502 + 0.395\times10^{-3}T + 0.062\times10^{-6}T^{2} + 141.450T^{-1}$

$\Delta Gf° = 9.502 - 0.395\times10^{-3}T\ln T - 0.062\times10^{-6}T^{2} + 70.725T^{-1} + 15.094\times10^{-3}T$

Source: Data from JANAF (60).

$NF_3(g)$

Nitrogen Trifluoride (ideal gas)

[Formation: $0.5N_2(g) + 1.5F_2(g) = NF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.756	62.300	62.300	0	-31.570	-21.657	15.875
300	12.799	62.379	62.300	.024	-31.573	-21.595	15.732
400	14.785	66.349	62.826	1.409	-31.691	-18.246	9.969
500	16.149	69.805	63.885	2.960	-31.697	-14.883	6.505
600	17.072	72.836	65.129	4.624	-31.635	-11.526	4.198
700	17.708	75.519	66.426	6.365	-31.529	-8.183	2.555
800	18.158	77.914	67.715	8.159	-31.399	-4.857	1.327
900	18.485	80.073	68.971	9.992	-31.253	-1.547	.376
1000	18.728	82.034	70.181	11.853	-31.099	1.744	-.381
1100	18.914	83.828	71.341	13.736	-30.939	5.022	-.998
1200	19.059	85.480	72.451	15.635	-30.777	8.283	-1.509
1300	19.174	87.010	73.512	17.547	-30.612	11.534	-1.939
1400	19.266	88.435	74.529	19.469	-30.451	14.767	-2.305
1500	19.342	89.767	75.501	21.399	-30.290	17.991	-2.621
1600	19.404	91.017	76.431	23.337	-30.129	21.205	-2.896
1700	19.456	92.195	77.324	25.280	-29.969	24.410	-3.138
1800	19.500	93.308	78.181	27.228	-29.814	27.605	-3.352
1900	19.537	94.364	79.006	29.180	-29.657	30.790	-3.542
2000	19.569	95.366	79.799	31.135	-29.507	33.968	-3.712

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 17.363 + 1.530\times10^{-3}T - 4.501\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 17.363\times10^{-3}T + 0.765\times10^{-6}T^2 + 4.501\times10^{2}T^{-1} - 6.754$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -33.006 + 1.342\times10^{-3}T + 0.209\times10^{-6}T^2 + 303.300T^{-1}$

$\Delta Gf^\circ = -33.006 - 1.342\times10^{-3}T\ln T - 0.209\times10^{-6}T^2 + 151.650T^{-1} + 44.072\times10^{-3}T$

Source: Data from Chase (24).

N_2F_2(g,cis)

Cis-Dinitrogen Difluoride, Cis-Difluorodiazine (ideal gas)

[Formation: $N_2(g) + F_2(g) = N_2F_2(g,cis)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	11.941	62.071	62.071	0	16.400	25.983	-19.046
300	11.982	62.145	62.072	.022	16.395	26.042	-18.971
400	13.900	65.867	62.564	1.321	16.228	29.288	-16.002
500	15.306	69.129	63.559	2.785	16.185	32.560	-14.232
600	16.318	72.014	64.732	4.369	16.226	35.832	-13.051
700	17.053	74.587	65.960	6.039	16.321	39.093	-12.205
800	17.595	76.902	67.186	7.773	16.450	42.336	-11.566
900	18.002	78.999	68.383	9.554	16.601	45.565	-11.065
1000	18.313	80.912	69.542	11.370	16.762	48.773	-10.659
1100	18.555	82.669	70.656	13.214	16.932	51.967	-10.325
1200	18.746	84.292	71.725	15.080	17.107	55.145	-10.043
1300	18.900	85.799	72.751	16.962	17.283	58.308	-9.802
1400	19.025	87.205	73.734	18.859	17.459	61.455	-9.593
1500	19.127	88.521	74.677	20.766	17.634	64.592	-9.411
1600	19.213	89.758	75.581	22.684	17.810	67.717	-9.250
1700	19.284	90.925	76.450	24.608	17.983	70.831	-9.106
1800	19.345	92.029	77.285	26.540	18.155	73.935	-8.977
1900	19.397	93.076	78.088	28.477	18.326	77.030	-8.860
2000	19.442	94.072	78.862	30.419	18.493	80.115	-8.754

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 16.183 + 2.192\times10^{-3}T - 4.352\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 16.183\times10^{-3}T + 1.096\times10^{-6}T^2 + 4.352\times10^{2}T^{-1} - 6.382$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = 14.876 + 1.158\times10^{-3}T + 0.333\times10^{-6}T^2 + 342.600T^{-1}$

$\Delta Gf^\circ = 14.876 - 1.158\times10^{-3}T\ln T - 0.333\times10^{-6}T^2 + 171.300T^{-1} + 42.023\times10^{-3}T$

Source: Data from JANAF (60).

N_2F_2(g,trans)

Trans-Dinitrogen Difluoride, Trans-Difluorodiazine (ideal gas)

[Formation: $N_2(g) + F_2(g) = N_2F_2(g,trans)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.779	62.752	62.752	0	19.400	28.780	-21.096
300	12.812	62.832	62.752	.024	19.397	28.838	-21.008
400	14.392	66.744	63.277	1.387	19.294	32.004	-17.486
500	15.583	70.090	64.312	2.889	19.289	35.184	-15.378
600	16.473	73.014	65.524	4.494	19.351	38.357	-13.971
700	17.139	75.605	66.782	6.176	19.458	41.517	-12.962
800	17.641	77.928	68.033	7.916	19.593	44.659	-12.200
900	18.026	80.029	69.250	9.701	19.748	47.785	-11.604
1000	18.323	81.945	70.426	11.519	19.911	50.889	-11.122
1100	18.558	83.702	71.554	13.363	20.081	53.980	-10.725
1200	18.744	85.325	72.634	15.229	20.256	57.054	-10.391
1300	18.895	86.832	73.670	17.111	20.432	60.115	-10.106
1400	19.019	88.237	74.661	19.007	20.607	63.159	-9.859
1500	19.121	89.553	75.610	20.914	20.782	66.192	-9.644
1600	19.206	90.789	76.520	22.830	20.956	69.214	-9.454
1700	19.277	91.956	77.394	24.755	21.130	72.225	-9.285
1800	19.338	93.060	78.235	26.685	21.300	75.224	-9.133
1900	19.390	94.107	79.043	28.622	21.471	78.216	-8.997
2000	19.435	95.102	79.820	30.563	21.637	81.199	-8.873

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 16.135 + 2.190\times10^{-3}T - 3.563\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 16.135\times10^{-3}T + 1.095\times10^{-6}T^2 + 3.563\times10^{2}T^{-1} - 6.103$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = 18.155 + 1.110\times10^{-3}T + 0.332\times10^{-6}T^2 + 263.700T^{-1}$

$\Delta Gf^\circ = 18.155 - 1.110\times10^{-3}T\ln T - 0.332\times10^{-6}T^2 + 131.850T^{-1} + 40.577\times10^{-3}T$

Source: Data from JANAF (60).

$N_2F_4(g)$

Dinitrogen Tetrafluoride, Tetrafluorohydrazine (ideal gas)

[Formation: $N_2(g) + 2F_2(g) = N_2F_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	18.922	71.962	71.962	0	-2.000	19.077	-13.984
300	19.000	72.079	71.962	.035	-2.006	19.208	-13.993
400	22.584	78.066	72.754	2.125	-2.151	26.310	-14.375
500	25.047	83.388	74.360	4.514	-2.073	33.419	-14.607
600	26.717	88.112	76.265	7.108	-1.852	40.498	-14.751
700	27.868	92.322	78.263	9.841	-1.542	47.534	-14.840
800	28.684	96.100	80.262	12.670	-1.180	54.518	-14.893
900	29.277	99.514	82.214	15.570	-.781	61.459	-14.924
1000	29.719	102.623	84.102	18.521	-.365	68.350	-14.938
1100	30.057	105.472	85.917	21.510	.064	75.202	-14.941
1200	30.320	108.099	87.657	24.530	.502	82.013	-14.936
1300	30.528	110.534	89.325	27.572	.943	88.790	-14.927
1400	30.696	112.803	90.922	30.634	1.384	95.528	-14.912
1500	30.833	114.925	92.452	33.710	1.825	102.238	-14.896
1600	30.946	116.919	93.919	36.800	2.267	108.918	-14.877
1700	31.040	118.798	95.328	39.899	2.707	115.572	-14.858
1800	31.120	120.575	96.682	43.007	3.143	122.197	-14.837
1900	31.188	122.259	97.984	46.123	3.580	128.801	-14.815
2000	31.246	123.860	99.238	49.244	4.009	135.379	-14.793

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 27.231 + 2.782\times10^{-3}T - 8.123\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 27.231\times10^{-3}T + 1.391\times10^{-6}T^2 + 8.123\times10^{2}T^{-1} - 10.967$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -5.220 + 3.698\times10^{-3}T + 0.454\times10^{-6}T^2 + 619.200T^{-1}$

$\Delta Gf^\circ = -5.220 - 3.698\times10^{-3}T\ln T - 0.454\times10^{-6}T^2 + 309.600T^{-1} + 99.215\times10^{-3}T$

Source: Data from JANAF (60).

NaBr(c,l)
Sodium Bromide

[Formation: $Na(c,l,g) + 0.5Br_2(l,g) = NaBr(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.280	20.750	20.750	0	-86.296	-83.393	61.128
300	12.289	20.826	20.750	.023	-86.301	-83.374	60.737
332.6	12.407	22.100	20.820	.426	-86.418	-83.050	54.571
332.6	12.407	22.100	20.820	.426	-89.951	-83.050	54.571
371	12.547	23.468	21.027	.906	-89.916	-82.258	48.456
371	12.547	23.468	21.027	.906	-90.538	-82.258	48.456
400	12.652	24.416	21.239	1.271	-90.518	-81.611	44.590
500	13.020	27.277	22.169	2.554	-90.417	-79.394	34.703
600	13.425	29.687	23.225	3.877	-90.259	-77.203	28.121
700	13.831	31.786	24.302	5.239	-90.050	-75.044	23.430
800	14.307	33.663	25.357	6.645	-89.786	-72.917	19.920
900	15.069	35.387	26.376	8.110	-89.461	-70.826	17.199
1000	16.495	37.041	27.360	9.681	-89.030	-68.778	15.031
1020	16.905	37.372	27.553	10.015	-88.925	-68.374	14.650
1020	16.260	43.519	27.553	16.285	-82.655	-68.374	14.650
1100	16.260	44.746	28.759	17.586	-82.272	-67.269	13.365
1177	16.260	45.846	29.841	18.838	-81.908	-66.227	12.297
1177	16.260	45.846	29.841	18.838	-105.193	-66.227	12.297
1200	16.260	46.161	30.151	19.212	-105.039	-65.470	11.924
1300	16.260	47.463	31.434	20.838	-104.361	-62.198	10.456
1400	16.260	48.668	32.622	22.464	-103.685	-58.980	9.207

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
1020 K, melting point of NaBr; ΔH° = 6.270 kcal/mol.
1177 K, boiling point of Na to monatomic gas; ΔH° = 23.285 kcal/mol.
1661 K, boiling point of NaBr to equilibrium mixture; ΔH° = 37 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1020 K: $Cp^\circ = 9.793 + 5.858\times10^{-3}T + 0.667\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 9.793\times10^{-3}T + 2.929\times10^{-6}T^2 - 0.667\times10^{2}T^{-1} - 2.956$

1020-1400 K: $Cp^\circ = 16.260$

$H^\circ - H^\circ_{298} = 16.260\times10^{-3}T - 0.300$

NaBr(c,l) - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -84.968 - 3.203\times10^{-3}T - 1.679\times10^{-6}T^2 - 66.700T^{-1}$

$\Delta Gf^\circ = -84.968 + 3.203\times10^{-3}T\ln T + 1.679\times10^{-6}T^2 - 33.350T^{-1} - 13.095\times10^{-3}T$

332.6-371 K: $\Delta Hf^\circ = -89.968 + 1.377\times10^{-3}T - 1.756\times10^{-6}T^2 - 82.400T^{-1}$

$\Delta Gf^\circ = -89.968 - 1.377\times10^{-3}T\ln T + 1.756\times10^{-6}T^2 - 41.200T^{-1} + 28.583\times10^{-3}T$

371-1020 K: $\Delta Hf^\circ = -90.356 - 1.676\times10^{-3}T + 2.993\times10^{-6}T^2 + 8.500T^{-1}$

$\Delta Gf^\circ = -90.356 + 1.676\times10^{-3}T\ln T - 2.993\times10^{-6}T^2 + 4.250T^{-1} + 12.999\times10^{-3}T$

1020-1177 K: $\Delta Hf^\circ = -87.701 + 4.791\times10^{-3}T + 0.064\times10^{-6}T^2 + 75.200T^{-1}$

$\Delta Gf^\circ = -87.701 - 4.791\times10^{-3}T\ln T - 0.064\times10^{-6}T^2 + 37.600T^{-1} + 52.176\times10^{-3}T$

1177-1400 K: $\Delta Hf^\circ = -113.164 + 6.828\times10^{-3}T - 0.032\times10^{-6}T^2 - 26.700T^{-1}$

$\Delta Gf^\circ = -113.164 - 6.828\times10^{-3}T\ln T + 0.032\times10^{-6}T^2 - 13.350T^{-1} + 88.137\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Low-temperature heat capacities and entropy at 298 K from Gardner (85). High-temperature data based on Gardner (86). Boiling data from Murgulescu (163).

NaBr(g)

Sodium Bromide (ideal gas)

[Formation: $Na(c,l,g) + 0.5Br_2(l,g) = NaBr(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.681	57.628	57.628	0	-34.200	-42.292	31.000
300	8.685	57.681	57.628	.016	-34.213	-42.341	30.845
332.6	8.733	58.579	57.678	.300	-34.448	-43.212	28.394
332.6	8.733	58.579	57.678	.300	-37.980	-43.212	28.394
371	8.790	59.540	57.822	.637	-38.088	-43.813	25.809
371	8.790	59.540	57.822	.637	-38.710	-43.813	25.809
400	8.833	60.203	57.971	.893	-38.800	-44.208	24.154
500	8.915	62.183	58.621	1.781	-39.095	-45.524	19.898
600	8.970	63.814	59.356	2.675	-39.366	-46.785	17.041
700	9.010	65.200	60.094	3.574	-39.619	-48.003	14.987
800	9.043	66.405	60.809	4.477	-39.859	-49.182	13.436
900	9.072	67.472	61.491	5.383	-40.092	-50.334	12.223
1000	9.098	68.429	62.138	6.291	-40.324	-51.460	11.246
1100	9.121	69.297	62.750	7.202	-40.560	-52.563	10.443
1177	9.139	69.915	63.199	7.905	-40.745	-53.394	9.914
1177	9.139	69.915	63.199	7.905	-64.030	-53.394	9.914
1200	9.144	70.092	63.330	8.115	-64.040	-53.188	9.687
1300	9.166	70.825	63.878	9.031	-64.072	-52.280	8.789
1400	9.187	71.505	64.399	9.948	-64.105	-51.372	8.019
1500	9.208	72.139	64.894	10.868	-64.136	-50.462	7.352
1600	9.228	72.734	65.365	11.790	-64.166	-49.549	6.768
1700	9.248	73.294	65.815	12.714	-64.194	-48.635	6.252
1800	9.268	73.823	66.246	13.639	-64.221	-47.719	5.794
1900	9.287	74.325	66.658	14.567	-64.246	-46.801	5.383
2000	9.307	74.802	67.054	15.497	-64.270	-45.883	5.014

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
371 K, melting point of Na; $\Delta H°$ = 0.622 kcal/mol.
1177 K, boiling point of Na to monatomic gas; $\Delta H°$ = 23.285 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.931 + 0.192\times10^{-3}T - 0.273\times10^{5}T^{-2}$

$H°- H°_{298} = 8.931\times10^{-3}T + 0.096\times10^{-6}T^2 + 0.273\times10^{2}T^{-1} - 2.763$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -32.678 - 4.065\times10^{-3}T - 4.512\times10^{-6}T^2 + 27.300T^{-1}$

$\Delta Gf° = -32.678 + 4.065\times10^{-3}T\ln T + 4.512\times10^{-6}T^2 + 13.650T^{-1} - 56.907\times10^{-3}T$

332.6-371 K: $\Delta Hf° = -37.679 + 0.515\times10^{-3}T - 4.589\times10^{-6}T^2 + 11.600T^{-1}$

$\Delta Gf° = -37.679 - 0.515\times10^{-3}T\ln T + 4.589\times10^{-6}T^2 + 5.800T^{-1} - 15.229\times10^{-3}T$

371-1177 K: $\Delta Hf° = -38.067 - 2.538\times10^{-3}T + 0.161\times10^{-6}T^2 + 102.500T^{-1}$

$\Delta Gf° = -38.067 + 2.538\times10^{-3}T\ln T - 0.161\times10^{-6}T^2 + 51.250T^{-1} - 30.813\times10^{-3}T$

1177-2000 K: $\Delta Hf° = -63.530 - 0.501\times10^{-3}T + 0.064\times10^{-6}T^2 + 0.600T^{-1}$

$\Delta Gf° = -63.530 + 0.501\times10^{-3}T\ln T - 0.064\times10^{-6}T^2 + 0.300T^{-1} + 5.148\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data from JANAF (60).

$(NaBr)_2(g)$

Dimeric Sodium Bromide (ideal gas)

[Formation: $2Na(c,l,g) + Br_2(l,g) = (NaBr)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	19.150	83.384	83.384	0	-116.300	-122.981	90.147
300	19.159	83.503	83.386	.035	-116.322	-123.022	89.620
332.6	19.258	85.485	83.497	.661	-116.734	-123.728	81.300
332.6	19.258	85.485	83.497	.661	-123.799	-123.728	81.300
371	19.375	87.600	83.811	1.406	-123.945	-123.716	72.878
371	19.375	87.600	83.811	1.406	-125.189	-123.716	72.878
400	19.463	89.062	84.139	1.969	-125.318	-123.595	67.528
500	19.608	93.422	85.576	3.923	-125.728	-123.116	53.813
600	19.688	97.005	87.192	5.888	-126.093	-122.558	44.641
700	19.737	100.044	88.815	7.860	-126.426	-121.945	38.072
800	19.768	102.682	90.388	9.835	-126.736	-121.282	33.132
900	19.790	105.011	91.885	11.813	-127.037	-120.581	29.281
1000	19.806	107.097	93.304	13.793	-127.337	-119.848	26.192
1100	19.817	108.986	94.646	15.774	-127.650	-119.088	23.660
1177	19.824	110.326	95.628	17.300	-127.899	-118.470	21.998
1177	19.824	110.326	95.628	17.300	-174.469	-118.470	21.998
1200	19.826	110.710	95.913	17.756	-174.453	-117.381	21.378
1300	19.833	112.298	97.114	19.739	-174.367	-112.625	18.934
1400	19.838	113.767	98.251	21.723	-174.283	-107.877	16.840
1500	19.843	115.136	99.331	23.707	-174.201	-103.140	15.027
1600	19.846	116.417	100.360	25.691	-174.120	-98.405	13.441
1700	19.849	117.620	101.340	27.676	-174.039	-93.677	12.043
1800	19.852	118.755	102.277	29.661	-173.959	-88.952	10.800
1900	19.854	119.828	103.172	31.646	-173.880	-84.229	9.688
2000	19.856	120.847	104.031	33.632	-173.802	-79.514	8.689

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
1177 K, boiling point of Na to monatomic gas; ΔH° = 23.285 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.861 + 0.006\times10^{-3}T - 0.633\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.861\times10^{-3}T + 0.003\times10^{-6}T^2 + 0.633\times10^{2}T^{-1} - 6.134$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -113.865 - 6.132\times10^{-3}T - 9.213\times10^{-6}T^2 + 63.300T^{-1}$

$\Delta Gf^\circ = -113.865 + 6.132\times10^{-3}T\ln T + 9.213\times10^{-6}T^2 + 31.650T^{-1} - 68.616\times10^{-3}T$

332.6-371 K: $\Delta Hf^\circ = -123.865 + 3.029\times10^{-3}T - 9.368\times10^{-6}T^2 + 31.900T^{-1}$

$\Delta Gf^\circ = -123.865 - 3.029\times10^{-3}T\ln T + 9.368\times10^{-6}T^2 + 15.950T^{-1} + 14.739\times10^{-3}T$

371-1177 K: $\Delta Hf^\circ = -124.642 - 3.077\times10^{-3}T + 0.132\times10^{-6}T^2 + 213.700T^{-1}$

$\Delta Gf^\circ = -124.642 + 3.077\times10^{-3}T\ln T - 0.132\times10^{-6}T^2 + 106.850T^{-1} - 16.429\times10^{-3}T$

1177-2000 K: $\Delta Hf^\circ = -175.568 + 0.997\times10^{-3}T - 0.060\times10^{-6}T^2 + 9.900T^{-1}$

$\Delta Gf^\circ = -175.568 - 0.997\times10^{-3}T\ln T + 0.060\times10^{-6}T^2 + 4.950T^{-1} + 55.492\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data from JANAF (60).

NaCl(c,l)
Sodium Chloride
[Formation: $Na(c,l,g) + 0.5Cl_2(g) = NaCl(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.070	17.240	17.240	0	-98.268	-91.797	67.288
300	12.080	17.315	17.242	.022	-98.265	-91.757	66.844
371	12.404	19.922	17.512	.894	-98.189	-90.226	53.150
371	12.404	19.922	17.512	.894	-98.811	-90.226	53.150
400	12.536	20.861	17.721	1.256	-98.791	-89.556	48.930
500	12.886	23.696	18.642	2.527	-98.687	-87.257	38.140
600	13.264	26.077	19.687	3.834	-98.535	-84.984	30.955
700	13.711	28.155	20.752	5.182	-98.332	-82.743	25.833
800	14.243	30.019	21.795	6.579	-98.073	-80.532	22.000
900	14.869	31.732	22.805	8.034	-97.754	-78.357	19.027
1000	15.591	33.335	23.779	9.556	-97.368	-76.222	16.658
1073.8	16.188	34.466	24.475	10.728	-97.040	-74.675	15.198
1073.8	16.360	40.761	24.475	17.488	-90.280	-74.675	15.198
1100	16.360	41.156	24.868	17.917	-90.152	-74.296	14.761
1177	16.360	42.262	25.970	19.177	-89.779	-73.194	13.591
1177	16.360	42.262	25.970	19.177	-113.064	-73.194	13.591
1200	16.360	42.579	26.285	19.553	-112.907	-72.419	13.189
1300	16.360	43.889	27.590	21.189	-112.218	-69.071	11.612
1400	16.360	45.101	28.797	22.825	-111.531	-65.778	10.268
1500	16.360	46.230	29.923	24.461	-110.845	-62.535	9.111
1600	16.360	47.286	30.975	26.097	-110.160	-59.337	8.105
1700	16.360	48.278	31.964	27.733	-109.476	-56.181	7.223
1800	16.360	49.213	32.897	29.369	-108.792	-53.067	6.443

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
1073.8 K, melting point of NaCl; ΔH° = 6.760 kcal/mol.
1177 K, boiling point of Na to monatomic gas; ΔH° = 23.285 kcal/mol.
1722 K, boiling point of NaCl to equilibrium mixture; ΔH° = 41 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1073.8 K: $Cp^\circ = 10.039 + 5.352\times10^{-3}T + 0.387\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 10.039\times10^{-3}T + 2.676\times10^{-6}T^2 - 0.387\times10^{2}T^{-1} - 3.101$

1073.8-1800 K: $Cp^\circ = 16.360$

$H^\circ - H^\circ_{298} = 16.360\times10^{-3}T - 0.079$

NaCl(c,l) - Continued

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf^\circ = -98.343 + 1.674\times10^{-3}T - 2.026\times10^{-6}T^2 - 72.850T^{-1}$

$\Delta Gf^\circ = -98.343 - 1.674\times10^{-3}T\ln T + 2.026\times10^{-6}T^2 - 36.425T^{-1} + 31.300\times10^{-3}T$

371-1073.8 K: $\Delta Hf^\circ = -98.731 - 1.379\times10^{-3}T + 2.724\times10^{-6}T^2 + 18.050T^{-1}$

$\Delta Gf^\circ = -98.731 + 1.379\times10^{-3}T\ln T - 2.724\times10^{-6}T^2 + 9.025T^{-1} + 15.716\times10^{-3}T$

1073.8-1177 K: $\Delta Hf^\circ = -95.709 + 4.942\times10^{-3}T + 0.048\times10^{-6}T^2 + 56.750T^{-1}$

$\Delta Gf^\circ = -95.709 - 4.942\times10^{-3}T\ln T - 0.048\times10^{-6}T^2 + 28.375T^{-1} + 54.126\times10^{-3}T$

1177-1800 K: $\Delta Hf^\circ = -121.172 + 6.979\times10^{-3}T - 0.048\times10^{-6}T^2 - 45.150T^{-1}$

$\Delta Gf^\circ = -121.172 - 6.979\times10^{-3}T\ln T + 0.048\times10^{-6}T^2 - 22.575T^{-1} + 90.086\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Low-temperature heat capacities and entropy at 298 K from Barron (8). High-temperature data based on Dawson (54). Boiling data from Murgulescu (163).

NaCl(g)
Sodium Chloride (ideal gas)
[Formation: $Na(c,l,g) + 0.5Cl_2(g) = NaCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.553	54.897	54.897	0	-42.220	-46.977	34.434
300	8.558	54.950	54.897	.016	-42.224	-47.006	34.243
371	8.694	56.785	55.089	.629	-42.407	-48.119	28.346
371	8.694	56.785	55.089	.629	-43.029	-48.119	28.346
400	8.749	57.441	55.236	.882	-43.117	-48.514	26.506
500	8.854	59.406	55.880	1.763	-43.403	-49.828	21.780
600	8.921	61.026	56.606	2.652	-43.670	-51.088	18.608
700	8.969	62.405	57.339	3.546	-43.921	-52.306	16.330
800	9.006	63.605	58.049	4.445	-44.160	-53.487	14.612
900	9.037	64.668	58.727	5.347	-44.393	-54.639	13.268
1000	9.064	65.622	59.370	6.252	-44.625	-55.766	12.187
1100	9.088	66.487	59.978	7.160	-44.861	-56.869	11.299
1177	9.105	67.102	60.423	7.861	-45.047	-57.699	10.714
1177	9.105	67.102	60.423	7.861	-68.332	-57.699	10.714
1200	9.110	67.278	60.553	8.070	-68.342	-57.493	10.471
1300	9.131	68.008	61.099	8.982	-68.377	-56.585	9.513
1400	9.152	68.686	61.617	9.896	-68.412	-55.678	8.692
1500	9.171	69.318	62.110	10.812	-68.446	-54.768	7.980
1600	9.190	69.910	62.579	11.730	-68.479	-53.854	7.356
1700	9.209	70.468	63.027	12.650	-68.511	-52.939	6.806
1800	9.227	70.995	63.455	13.572	-68.541	-52.023	6.316
1900	9.245	71.494	63.865	14.496	-68.570	-51.102	5.878
2000	9.263	71.969	64.258	15.421	-68.600	-50.184	5.484

Phase changes: 371 K, melting point of Na; $\Delta H°$ = 0.622 kcal/mol.
1177 K, boiling point of Na to monatomic gas; $\Delta H°$ = 23.285 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.910 + 0.186\times10^{-3}T - 0.367\times10^{5}T^{-2}$

$H°- H°_{298} = 8.910\times10^{-3}T + 0.093\times10^{-6}T^2 + 0.367\times10^{2}T^{-1} - 2.788$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -41.981 + 0.545\times10^{-3}T - 4.609\times10^{-6}T^2 + 2.550T^{-1}$

$\Delta Gf° = -41.981 - 0.545\times10^{-3}T\ln T + 4.609\times10^{-6}T^2 + 1.275T^{-1} - 15.034\times10^{-3}T$

371-1177 K: $\Delta Hf° = -42.370 - 2.508\times10^{-3}T + 0.141\times10^{-6}T^2 + 93.450T^{-1}$

$\Delta Gf° = -42.370 + 2.508\times10^{-3}T\ln T - 0.141\times10^{-6}T^2 + 46.725T^{-1} - 30.618\times10^{-3}T$

1177-2000 K: $\Delta Hf° = -67.833 - 0.471\times10^{-3}T + 0.045\times10^{-6}T^2 - 8.450T^{-1}$

$\Delta Gf° = -67.833 + 0.471\times10^{-3}T\ln T - 0.045\times10^{-6}T^2 - 4.225T^{-1} + 5.342\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data from JANAF (60).

$(NaCl)_2(g)$

Dimeric Sodium Chloride (ideal gas)

[Formation: $2Na(c,l,g) + Cl_2(g) = (NaCl)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	18.831	77.757	77.757	0	-136.500	-136.462	100.028
300	18.843	77.873	77.757	.035	-136.504	-136.460	99.410
371	19.152	81.916	78.178	1.387	-136.745	-136.426	80.365
371	19.152	81.916	78.178	1.387	-137.989	-136.426	80.365
400	19.278	83.362	78.502	1.944	-138.113	-136.299	74.469
500	19.487	87.689	79.923	3.883	-138.509	-135.798	59.356
600	19.603	91.253	81.523	5.838	-138.865	-135.222	49.254
700	19.674	94.281	83.135	7.802	-139.191	-134.591	42.021
800	19.720	96.911	84.696	9.772	-139.497	-133.912	36.583
900	19.752	99.235	86.184	11.746	-139.793	-133.194	32.344
1000	19.775	101.318	87.596	13.722	-140.091	-132.447	28.946
1100	19.792	103.203	88.929	15.701	-140.401	-131.669	26.160
1177	19.801	104.543	89.908	17.225	-140.650	-131.043	24.332
1177	19.801	104.543	89.908	17.225	-187.220	-131.043	24.332
1200	19.804	104.926	90.193	17.680	-187.204	-129.950	23.667
1300	19.814	106.512	91.388	19.661	-187.117	-125.177	21.044
1400	19.822	107.980	92.521	21.643	-187.033	-120.415	18.797
1500	19.829	109.348	93.597	23.626	-186.950	-115.662	16.852
1600	19.834	110.628	94.622	25.609	-186.869	-110.912	15.150
1700	19.839	111.831	95.600	27.593	-186.788	-106.167	13.649
1800	19.842	112.965	96.533	29.577	-186.709	-101.429	12.315
1900	19.845	114.038	97.427	31.561	-186.631	-96.691	11.122
2000	19.848	115.056	98.283	33.546	-186.555	-91.959	10.049

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.

1177 K, boiling point of Na to monatomic gas; ΔH° = 23.285 cal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.841 + 0.020\times10^{-3}T - 0.903\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.841\times10^{-3}T + 0.010\times10^{-6}T^2 + 0.903\times10^{2}T^{-1} - 6.219$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf^\circ = -136.667 + 3.112\times10^{-3}T - 9.394\times10^{-6}T^2 + 22.000T^{-1}$

$\Delta Gf^\circ = -136.667 - 3.112\times10^{-3}T\ln T + 9.394\times10^{-6}T^2 + 11.000T^{-1} + 15.494\times10^{-3}T$

371-1177 K: $\Delta Hf^\circ = -137.443 - 2.994\times10^{-3}T + 0.106\times10^{-6}T^2 + 203.800T^{-1}$

$\Delta Gf^\circ = -137.443 + 2.994\times10^{-3}T\ln T - 0.106\times10^{-6}T^2 + 101.900T^{-1} - 15.674\times10^{-3}T$

1177-2000 K: $\Delta Hf^\circ = -188.369 + 1.080\times10^{-3}T - 0.086\times10^{-6}T^2$

$\Delta Gf^\circ = -188.369 - 1.080\times10^{-3}T\ln T + 0.086\times10^{-6}T^2 + 56.248\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data from JANAF (60).

NaF(c,l)
Sodium Fluoride
[Formation: $Na(c,l,g) + 0.5F_2(g) = NaF(c,l)$]

T, K	cal/mol-K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	11.210	12.260	12.260	0	-137.105	-129.872	95.198
300	11.233	12.329	12.260	.021	-137.103	-129.826	94.577
371	11.800	14.787	12.514	.843	-137.055	-128.110	75.466
371	11.800	14.787	12.514	.843	-137.677	-128.110	75.466
400	12.031	15.684	12.712	1.189	-137.663	-127.363	69.587
500	12.496	18.421	13.589	2.416	-137.579	-124.796	54.548
600	12.865	20.733	14.591	3.685	-137.447	-122.251	44.529
700	13.220	22.743	15.616	4.989	-137.272	-119.733	37.382
800	13.594	24.532	16.621	6.329	-137.059	-117.242	32.029
900	14.004	26.156	17.590	7.709	-136.804	-114.778	27.872
1000	14.457	27.655	18.523	9.132	-136.511	-112.347	24.553
1100	14.960	29.056	19.418	10.602	-136.180	-109.947	21.844
1177	15.387	30.082	20.082	11.770	-135.895	-108.117	20.075
1177	15.387	30.082	20.082	11.770	-159.180	-108.117	20.075
1200	15.515	30.381	20.277	12.125	-159.044	-107.123	19.509
1269	15.929	31.260	20.850	13.210	-158.609	-104.146	17.936
1269	16.670	37.588	20.850	21.240	-150.579	-104.146	17.936
1300	16.670	37.990	21.254	21.757	-150.355	-103.014	17.318
1400	16.670	39.225	22.494	23.424	-149.635	-99.400	15.517
1500	16.670	40.376	23.649	25.091	-148.917	-95.840	13.964
1600	16.670	41.451	24.727	26.758	-148.200	-92.323	12.611
1700	16.670	42.462	25.741	28.425	-147.484	-88.853	11.423
1800	16.670	43.415	26.697	30.092	-146.770	-85.425	10.372

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 cal/mol.
1269 K, melting point of NaF; ΔH° = 8.030 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1269 K: $Cp^\circ = 10.767 + 3.834\times10^{-3}T - 0.621\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 10.767\times10^{-3}T + 1.917\times10^{-6}T^2 + 0.621\times10^{2}T^{-1} - 3.589$

1269-1800 K: $Cp^\circ = 16.670$
$H^\circ - H^\circ_{298} = 16.670\times10^{-3}T + 0.086$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf^\circ = -137.657 + 2.562\times10^{-3}T - 2.828\times10^{-6}T^2 + 11.850T^{-1}$
$\Delta Gf^\circ = -137.657 - 2.562\times10^{-3}T\ln T + 2.828\times10^{-6}T^2 + 5.925T^{-1} + 39.799\times10^{-3}T$

371-1177 K: $\Delta Hf^\circ = -138.045 - 0.491\times10^{-3}T + 1.922\times10^{-6}T^2 + 102.750T^{-1}$
$\Delta Gf^\circ = -138.045 + 0.491\times10^{-3}T\ln T - 1.922\times10^{-6}T^2 + 51.375T^{-1} + 24.215\times10^{-3}T$

1177-1269 K: $\Delta Hf^\circ = -163.508 + 1.546\times10^{-3}T + 1.826\times10^{-6}T^2 + 0.850T^{-1}$
$\Delta Gf^\circ = -163.508 - 1.546\times10^{-3}T\ln T - 1.826\times10^{-6}T^2 + 0.425T^{-1} + 60.176\times10^{-3}T$

1269-1800 K: $\Delta Hf^\circ = -159.833 + 7.449\times10^{-3}T - 0.091\times10^{-6}T^2 - 61.250T^{-1}$
$\Delta Gf^\circ = -159.833 - 7.449\times10^{-3}T\ln T + 0.091\times10^{-6}T^2 - 30.625T^{-1} + 97.049\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Low-temperature heat capacities and entropy at 298 K from King (126). High-temperature data based on O'Brien (173) and Holm (102).

NaF(g)
Sodium Fluoride (ideal gas)
[Formation: $Na(c,l,g) + 0.5F_2(g) = NaF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.178	51.983	51.983	0	-69.600	-74.210	54.397
300	8.185	52.034	51.984	.015	-69.604	-74.239	54.082
371	8.404	53.799	52.166	.606	-69.787	-75.316	44.367
371	8.404	53.799	52.166	.606	-70.409	-75.316	44.367
400	8.494	54.435	52.308	.851	-70.496	-75.696	41.358
500	8.674	56.351	52.931	1.710	-70.781	-76.962	33.640
600	8.789	57.943	53.638	2.583	-71.043	-78.174	28.475
700	8.868	59.304	54.353	3.466	-71.290	-79.344	24.772
800	8.926	60.493	55.048	4.356	-71.526	-80.478	21.985
900	8.972	61.547	55.713	5.251	-71.757	-81.583	19.811
1000	9.010	62.494	56.344	6.150	-71.988	-82.662	18.066
1100	9.043	63.354	56.942	7.053	-72.224	-83.719	16.633
1177	9.065	63.967	57.382	7.750	-72.409	-84.513	15.692
1177	9.065	63.967	57.382	7.750	-95.694	-84.513	15.692
1200	9.071	64.142	57.509	7.959	-95.704	-84.297	15.352
1300	9.097	64.870	58.049	8.867	-95.740	-83.343	14.011
1400	9.121	65.545	58.561	9.778	-95.776	-82.389	12.861
1500	9.144	66.175	59.048	10.691	-95.812	-81.433	11.865
1600	9.166	66.766	59.512	11.607	-95.846	-80.473	10.992
1700	9.186	67.322	59.955	12.524	-95.880	-79.511	10.222
1800	9.206	67.848	60.379	13.444	-95.912	-78.548	9.537
1900	9.226	68.346	60.785	14.366	-95.944	-77.580	8.924
2000	9.244	68.820	61.175	15.289	-95.977	-76.615	8.372

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
1177 K, boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.813 + 0.244\times10^{-3}T - 0.629\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.813\times10^{-3}T + 0.122\times10^{-6}T^2 + 0.629\times10^{2}T^{-1} - 2.849$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf^\circ = -69.413 + 0.608\times10^{-3}T - 4.623\times10^{-6}T^2 + 12.650T^{-1}$

$\Delta Gf^\circ = -69.413 - 0.608\times10^{-3}T\ln T + 4.623\times10^{-6}T^2 + 6.325T^{-1} - 14.077\times10^{-3}T$

371-1177 K: $\Delta Hf^\circ = -69.801 - 2.445\times10^{-3}T + 0.127\times10^{-6}T^2 + 103.550T^{-1}$

$\Delta Gf^\circ = -69.801 + 2.445\times10^{-3}T\ln T - 0.127\times10^{-6}T^2 + 51.775T^{-1} - 29.661\times10^{-3}T$

1177-2000 K: $\Delta Hf^\circ = -95.264 - 0.408\times10^{-3}T + 0.031\times10^{-6}T^2 + 1.650T^{-1}$

$\Delta Gf^\circ = -95.264 + 0.408\times10^{-3}T\ln T - 0.031\times10^{-6}T^2 + 0.825T^{-1} + 6.300\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data from JANAF (60).

$(NaF)_2(g)$

Dimeric Sodium Fluoride (ideal gas)

[Formation: $2Na(c,l,g) + F_2(g) = (NaF)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	16.926	68.655	68.655	0	-198.200	-196.893	144.325
300	16.956	68.760	68.657	.031	-198.207	-196.884	143.428
371	17.763	72.463	69.039	1.270	-198.516	-196.538	115.776
371	17.763	72.463	69.039	1.270	-199.760	-196.538	115.776
400	18.092	73.812	69.337	1.790	-199.905	-196.281	107.242
500	18.687	77.920	70.656	3.632	-200.349	-195.321	85.374
600	19.031	81.360	72.162	5.519	-200.734	-194.280	70.765
700	19.245	84.311	73.691	7.434	-201.079	-193.178	60.312
800	19.388	86.891	75.184	9.366	-201.399	-192.027	52.459
900	19.487	89.180	76.613	11.310	-201.706	-190.835	46.340
1000	19.559	91.237	77.974	13.263	-202.013	-189.611	41.439
1100	19.612	93.104	79.267	15.221	-202.333	-188.359	37.423
1177	19.644	94.432	80.215	16.733	-202.587	-187.364	34.790
1177	19.644	94.432	80.215	16.733	-249.157	-187.364	34.790
1200	19.653	94.812	80.491	17.185	-249.142	-186.160	33.904
1300	19.685	96.387	81.655	19.152	-249.062	-180.910	30.413
1400	19.711	97.847	82.760	21.122	-248.986	-175.672	27.423
1500	19.731	99.207	83.811	23.094	-248.911	-170.440	24.833
1600	19.748	100.481	84.814	25.068	-248.837	-165.210	22.566
1700	19.762	101.679	85.771	27.043	-248.764	-159.987	20.567
1800	19.774	102.809	86.687	29.020	-248.693	-154.767	18.791
1900	19.784	103.878	87.563	30.998	-248.622	-149.548	17.202
2000	19.792	104.893	88.404	32.977	-248.554	-144.336	15.772

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 371 K, melting point of Na; $\Delta H° = 0.622$ kcal/mol.
1177 K, boiling point of Na to monatomic gas; $\Delta H° = 23.285$ cal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.580 + 0.182\times10^{-3}T - 2.408\times10^{5}T^{-2}$

$H°- H°_{298} = 19.580\times10^{-3}T + 0.091\times10^{-6}T^2 + 2.408\times10^{2}T^{-1} - 6.654$

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf° = -198.780 + 3.170\times10^{-3}T - 9.399\times10^{-6}T^2 + 140.300T^{-1}$

$\Delta Gf° = -198.780 - 3.170\times10^{-3}T\ln T + 9.399\times10^{-6}T^2 + 70.150T^{-1} + 20.800\times10^{-3}T$

371-1177 K: $\Delta Hf° = -199.556 - 2.936\times10^{-3}T + 0.101\times10^{-6}T^2 + 322.100T^{-1}$

$\Delta Gf° = -199.556 + 2.936\times10^{-3}T\ln T - 0.101\times10^{-6}T^2 + 161.050T^{-1} - 10.368\times10^{-3}T$

1177-2000 K: $\Delta Hf° = -250.482 + 1.138\times10^{-3}T - 0.091\times10^{-6}T^2 + 118.300T^{-1}$

$\Delta Gf° = -250.482 - 1.138\times10^{-3}T\ln T + 0.091\times10^{-6}T^2 + 59.150T^{-1} + 61.553\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data are those estimated by JANAF (60).

NaI(c,l)
Sodium Iodide
[Formation: $Na(c,l,g) + 0.5I_2(c,l,g) = NaI(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.450	23.550	23.550	0	-68.780	-67.997	49.842
300	12.459	23.627	23.550	.023	-68.781	-67.991	49.531
371	12.756	26.305	23.830	.918	-68.874	-67.796	39.937
371	12.756	26.305	23.830	.918	-69.496	-67.796	39.937
386.8	12.823	26.839	23.942	1.120	-69.532	-67.723	38.264
386.8	12.823	26.839	23.942	1.120	-71.387	-67.723	38.264
400	12.878	27.270	24.045	1.290	-71.444	-67.597	36.933
458.4	13.096	29.040	24.570	2.049	-71.683	-67.017	31.951
458.4	13.096	29.040	24.570	2.049	-76.693	-67.017	31.951
500	13.252	30.184	24.990	2.597	-76.637	-66.140	28.910
600	13.660	32.635	26.065	3.942	-76.461	-64.057	23.332
700	14.191	34.778	27.159	5.333	-76.226	-62.008	19.360
800	14.936	36.719	28.235	6.787	-75.918	-59.996	16.390
900	15.988	38.535	29.279	8.330	-75.517	-58.029	14.091
934	16.432	39.136	29.628	8.880	-75.355	-57.373	13.425
934	16.040	45.212	29.628	14.555	-69.680	-57.373	13.425
1000	16.040	46.308	30.694	15.614	-69.375	-56.514	12.351
1100	16.040	47.836	32.183	17.218	-68.921	-55.250	10.977
1177	16.040	48.922	33.244	18.453	-68.575	-54.302	10.083
1177	16.040	48.922	33.244	18.453	-91.860	-54.302	10.083
1200	16.040	49.232	33.547	18.822	-91.712	-53.571	9.757
1300	16.040	50.516	34.804	20.426	-91.059	-50.417	8.476
1400	16.040	51.705	35.969	22.030	-90.408	-47.316	7.386

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
934 K, melting point of NaI; ΔH° = 5.675 kcal/mol.
1177 K, boiling point of Na to monatomic gas; ΔH° = 23.285 cal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-934 K: $Cp^\circ = 10.027 + 6.076\times10^{-3}T + 0.544\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 10.027\times10^{-3}T + 3.038\times10^{-6}T^2 - 0.544\times10^{2}T^{-1} - 3.077$

934-1400 K: $Cp^\circ = 16.040$

$H^\circ - H^\circ_{298} = 16.040\times10^{-3}T - 0.426$

NaI(c,l) - Continued

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf^\circ = -68.279 - 0.362\times10^{-3}T - 2.366\times10^{-6}T^2 - 54.400T^{-1}$

$\Delta Gf^\circ = -68.279 + 0.362\times10^{-3}T\ln T + 2.366\times10^{-6}T^2 - 27.200T^{-1} - 1.518\times10^{-3}T$

371-386.8 K: $\Delta Hf^\circ = -68.667 - 3.415\times10^{-3}T + 2.384\times10^{-6}T^2 + 36.500T^{-1}$

$\Delta Gf^\circ = -68.667 + 3.415\times10^{-3}T\ln T - 2.384\times10^{-6}T^2 + 18.250T^{-1} - 17.102\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -69.395 - 6.617\times10^{-3}T + 3.130\times10^{-6}T^2 + 36.500T^{-1}$

$\Delta Gf^\circ = -69.395 + 6.617\times10^{-3}T\ln T - 3.130\times10^{-6}T^2 + 18.250T^{-1} - 34.009\times10^{-3}T$

458.4-934 K: $\Delta Hf^\circ = -76.751 - 1.447\times10^{-3}T + 3.096\times10^{-6}T^2 + 28.850T^{-1}$

$\Delta Gf^\circ = -76.751 + 1.447\times10^{-3}T\ln T - 3.096\times10^{-6}T^2 + 14.425T^{-1} + 13.722\times10^{-3}T$

934-1177 K: $\Delta Hf^\circ = -74.101 + 4.566\times10^{-3}T + 0.058\times10^{-6}T^2 + 83.250T^{-1}$

$\Delta Gf^\circ = -74.101 - 4.566\times10^{-3}T\ln T - 0.058\times10^{-6}T^2 + 41.625T^{-1} + 49.141\times10^{-3}T$

1177-1400 K: $\Delta Hf^\circ = -99.564 + 6.603\times10^{-3}T - 0.038\times10^{-6}T^2 - 18.650T^{-1}$

$\Delta Gf^\circ = -99.564 - 6.603\times10^{-3}T\ln T + 0.038\times10^{-6}T^2 - 9.325T^{-1} + 85.102\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Low-temperature heat capacity and entropy at 298 K from Gardner (85). High-temperature data based on Gardner (86).

NaI(g)

Sodium Iodide (ideal gas)

[Formation: $Na(c,l,g) + 0.5I_2(c,l,g) = NaI(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.762	59.496	59.496	0	-20.260	-30.194	22.133
300	8.765	59.550	59.497	.016	-20.268	-30.255	22.041
371	8.848	61.422	59.692	.642	-20.631	-32.581	19.193
371	8.848	61.422	59.692	.642	-21.253	-32.581	19.193
386.8	8.867	61.791	59.770	.782	-21.351	-33.061	18.680
386.8	8.867	61.791	59.770	.782	-23.205	-33.061	18.680
400	8.882	62.089	59.841	.899	-23.315	-33.396	18.246
458.4	8.921	63.303	60.207	1.419	-23.792	-34.833	16.607
458.4	8.921	63.303	60.207	1.419	-28.803	-34.833	16.607
500	8.949	64.079	60.497	1.791	-28.923	-35.374	15.462
600	8.994	65.715	61.235	2.688	-29.196	-36.639	13.346
700	9.029	67.104	61.977	3.589	-29.450	-37.860	11.820
800	9.059	68.312	62.696	4.493	-29.691	-39.045	10.666
900	9.085	69.380	63.379	5.401	-29.926	-40.199	9.761
1000	9.109	70.339	64.029	6.310	-30.159	-41.328	9.032
1100	9.132	71.208	64.642	7.223	-30.396	-42.434	8.431
1177	9.149	71.827	65.092	7.927	-30.582	-43.267	8.034
1177	9.149	71.827	65.092	7.927	-53.867	-43.267	8.034
1200	9.154	72.004	65.223	8.137	-53.877	-43.063	7.843
1300	9.175	72.737	65.773	9.053	-53.912	-42.157	7.087
1400	9.196	73.418	66.295	9.972	-53.946	-41.252	6.440
1500	9.217	74.053	66.791	10.893	-53.978	-40.345	5.878
1600	9.237	74.649	67.265	11.815	-54.010	-39.436	5.387
1700	9.257	75.209	67.715	12.740	-54.040	-38.523	4.952
1800	9.277	75.739	68.146	13.667	-54.069	-37.610	4.566
1900	9.296	76.241	68.559	14.595	-54.097	-36.695	4.221
2000	9.316	76.718	68.955	15.526	-54.123	-35.777	3.909

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
1177 K, boiling point of Na to monatomic gas; ΔH° = 23.285 cal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.932 + 0.196\times10^{-3}T - 0.203\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.932\times10^{-3}T + 0.098\times10^{-6}T^2 + 0.203\times10^{2}T^{-1} - 2.740$

NaI(g) - Continued

Formation equations (kcal/mol):

298.15-371 K: $\Delta Hf^\circ = -19.422 - 1.458\times10^{-3}T - 5.306\times10^{-6}T^2 + 20.300T^{-1}$

$\Delta Gf^\circ = -19.422 + 1.458\times10^{-3}T\ln T + 5.306\times10^{-6}T^2 + 10.150T^{-1} - 46.131\times10^{-3}T$

371-386.8 K: $\Delta Hf^\circ = -19.810 - 4.511\times10^{-3}T - 0.556\times10^{-6}T^2 + 111.200T^{-1}$

$\Delta Gf^\circ = -19.810 + 4.511\times10^{-3}T\ln T + 0.556\times10^{-6}T^2 + 55.600T^{-1} - 61.714\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -20.538 - 7.713\times10^{-3}T + 0.190\times10^{-6}T^2 + 111.200T^{-1}$

$\Delta Gf^\circ = -20.538 + 7.713\times10^{-3}T\ln T - 0.190\times10^{-6}T^2 + 55.600T^{-1} - 78.622\times10^{-3}T$

458.4-1177 K: $\Delta Hf^\circ = -27.894 - 2.543\times10^{-3}T + 0.156\times10^{-6}T^2 + 103.550T^{-1}$

$\Delta Gf^\circ = -27.894 + 2.543\times10^{-3}T\ln T - 0.156\times10^{-6}T^2 + 51.775T^{-1} - 30.891\times10^{-3}T$

1177-2000 K: $\Delta Hf^\circ = -53.357 - 0.506\times10^{-3}T + 0.060\times10^{-6}T^2 + 1.650T^{-1}$

$\Delta Gf^\circ = -53.357 + 0.506\times10^{-3}T\ln T - 0.060\times10^{-6}T^2 + 0.825T^{-1} + 5.070\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Work (267). Other data from Wilkens (265).

$NbBr_5$(c,l,g)
Niobium Pentabromide
[Formation: $Nb(c) + 2.5Br_2(l,g) = NbBr_5(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	35.350	61.850	61.850	0	-132.900	-121.631	89.157
300	35.350	62.069	61.852	.065	-132.928	-121.559	88.554
332.6	35.350	65.716	62.055	1.217	-133.439	-120.298	79.046
332.6	35.350	65.716	62.055	1.217	-151.101	-120.298	79.046
400	35.350	72.238	63.238	3.600	-150.598	-114.113	62.347
500	35.350	80.126	65.856	7.135	-149.883	-105.076	45.928
527	35.350	81.985	66.634	8.090	-149.694	-102.661	42.574
527	51.100	92.877	66.634	13.830	-143.954	-102.661	42.574
600	49.330	99.405	70.238	17.500	-142.361	-97.046	35.349
634.6	48.340	102.144	71.904	19.190	-141.660	-94.454	32.528
634.6	31.377	130.666	71.904	37.290	-123.560	-94.454	32.528
700	31.455	133.748	77.538	39.347	-123.380	-91.466	28.556
800	31.533	137.954	84.833	42.497	-123.111	-86.923	23.746
900	31.588	141.671	90.945	45.653	-122.855	-82.414	20.013
1000	31.627	145.002	96.188	48.814	-122.608	-77.935	17.032
1100	31.656	148.017	100.764	51.978	-122.373	-73.480	14.599
1200	31.678	150.773	104.819	55.145	-122.146	-69.026	12.571
1300	31.695	153.309	108.452	58.314	-121.934	-64.603	10.861
1400	31.709	155.658	111.741	61.484	-121.736	-60.203	9.398
1500	31.720	157.846	114.743	64.655	-121.558	-55.814	8.132
1600	31.729	159.894	117.501	67.828	-121.396	-51.431	7.025
1700	31.736	161.818	120.053	71.001	-121.253	-47.062	6.050
1800	31.742	163.632	122.424	74.175	-121.129	-42.702	5.185
1900	31.748	165.348	124.638	77.349	-121.025	-38.357	4.412
2000	31.752	166.977	126.715	80.524	-120.945	-34.004	3.716

*Data for $NbBr_5$(c,l) estimated except enthalpy of formation at 298 K and temperature of fusion.

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
527 K, melting point of $NbBr_5$; $\Delta H°$ = 5.740 kcal/mol.
634.6 K, boiling point of $NbBr_5$; $\Delta H°$ = 18.100 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-527 K: $Cp° = 35.351$
$H°- H°_{298} = 35.351\times10^{-3}T - 10.540$

527-634.6 K: $Cp° = 65.252 - 26.580\times10^{-3}T$
$H°- H°_{298} = 65.252\times10^{-3}T - 13.290\times10^{-6}T^2 - 16.867$

634.6-2000 K: $Cp° = 31.845 - 0.030\times10^{-3}T - 1.809\times10^{5}T^{-2}$
$H°- H°_{298} = 31.845\times10^{-3}T - 0.015\times10^{-6}T^2 + 1.809\times10^{2}T^{-1} + 16.802$

$NbBr_5$(c,l,g) - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -128.429 - 15.073\times10^{-3}T - 0.522\times10^{-6}T^2 + 20.600T^{-1}$

$\Delta Gf^\circ = -128.429 + 15.073\times10^{-3}T\ln T + 0.522\times10^{-6}T^2 + 10.300T^{-1} - 63.347\times10^{-3}T$

332.6-527 K: $\Delta Hf^\circ = -153.430 + 7.830\times10^{-3}T - 0.910\times10^{-6}T^2 - 57.900T^{-1}$

$\Delta Gf^\circ = -153.430 - 7.830\times10^{-3}T\ln T + 0.910\times10^{-6}T^2 - 28.950T^{-1} + 145.040\times10^{-3}T$

527-634.6 K: $\Delta Hf^\circ = -159.757 + 37.731\times10^{-3}T - 14.200\times10^{-6}T^2 - 57.900T^{-1}$

$\Delta Gf^\circ = -159.757 - 37.731\times10^{-3}T\ln T + 14.200\times10^{-6}T^2 - 28.950T^{-1} + 337.437\times10^{-3}T$

634.6-2000 K: $\Delta Hf^\circ = -126.088 + 4.324\times10^{-3}T - 0.925\times10^{-6}T^2 + 123.000T^{-1}$

$\Delta Gf^\circ = -126.088 - 4.324\times10^{-3}T\ln T + 0.925\times10^{-6}T^2 + 61.500T^{-1} + 77.006\times10^{-3}T$

Source: Data from Chase (26) who estimated data for (c, l) except enthalpy of formation at 298 K and temperature of fusion.

$NbBr_5(g)$

Niobium Pentabromide (ideal gas)

[Formation: $Nb(c) + 2.5Br_2(l,g) = NbBr_5(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	30.068	107.348	107.348	0	-106.020	-108.316	79.397
300	30.087	107.534	107.348	.056	-106.057	-108.327	78.915
332.6	30.317	110.650	107.521	1.041	-106.736	-108.540	71.320
332.6	30.317	110.650	107.521	1.041	-124.398	-108.540	71.320
400	30.793	116.299	108.539	3.104	-124.215	-105.353	57.562
500	31.141	123.212	110.806	6.203	-123.935	-100.671	44.003
600	31.335	128.908	113.363	9.327	-123.655	-96.041	34.983
700	31.455	133.748	115.938	12.467	-123.380	-91.466	28.556
800	31.533	137.954	118.433	15.617	-123.112	-86.923	23.746
900	31.588	141.671	120.812	18.773	-122.855	-82.414	20.013
1000	31.627	145.002	123.068	21.934	-122.608	-77.935	17.032
1100	31.656	148.017	125.201	25.098	-122.373	-73.480	14.599
1200	31.678	150.773	127.219	28.265	-122.146	-69.026	12.571
1300	31.695	153.309	129.129	31.434	-121.934	-64.603	10.861
1400	31.709	155.658	130.941	34.604	-121.736	-60.203	9.398
1500	31.720	157.846	132.663	37.775	-121.558	-55.814	8.132
1600	31.729	159.894	134.301	40.948	-121.396	-51.431	7.025
1700	31.736	161.818	135.864	44.121	-121.254	-47.062	6.050
1800	31.742	163.632	137.357	47.295	-121.129	-42.702	5.185
1900	31.748	165.348	138.785	50.469	-121.025	-38.357	4.412
2000	31.752	166.977	140.155	53.644	-120.945	-34.004	3.716

Phase change: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 31.708 + 0.054\times10^{-3}T - 1.472\times10^{5}T^{-2}$

$H°- H°_{298} = 31.708\times10^{-3}T + 0.027\times10^{-6}T^2 + 1.472\times10^{2}T^{-1} - 9.950$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -100.959 - 18.716\times10^{-3}T - 0.495\times10^{-6}T^2 + 167.800T^{-1}$

$\Delta Gf° = -100.959 + 18.716\times10^{-3}T\ln T + 0.495\times10^{-6}T^2 + 83.900T^{-1} - 132.401\times10^{-3}T$

332.6-2000 K: $\Delta Hf° = -125.960 + 4.187\times10^{-3}T - 0.883\times10^{-6}T^2 + 89.300T^{-1}$

$\Delta Gf° = -125.960 - 4.187\times10^{-3}T\ln T + 0.883\times10^{-6}T^2 + 44.650T^{-1} + 75.987\times10^{-3}T$

Source: Data from Chase (26).

$NbCl_5$(c,l,g)

Niobium Pentachloride

[Formation: $Nb(c) + 2.5Cl_2(g) = NbCl_5(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	35.350	51.160	51.160	0	-190.570	-163.508	119.853
300	35.350	51.379	51.162	.065	-190.553	-163.340	118.992
400	35.350	61.548	52.548	3.600	-189.693	-154.404	84.361
478.9	35.350	67.912	54.571	6.389	-189.068	-147.501	67.312
478.9	52.180	84.819	54.571	14.486	-180.971	-147.501	67.312
500	51.760	87.061	55.895	15.583	-180.458	-146.037	63.832
519.7	51.281	89.052	57.114	16.598	-179.990	-144.690	60.846
519.7	30.534	113.031	57.114	29.060	-167.528	-144.690	60.846
600	30.846	117.444	64.901	31.526	-167.311	-141.175	51.422
700	31.088	122.218	72.757	34.623	-167.042	-136.846	42.725
800	31.249	126.381	79.205	37.741	-166.783	-132.551	36.211
900	31.361	130.068	84.655	40.872	-166.529	-128.283	31.151
1000	31.442	133.377	89.365	44.012	-166.288	-124.050	27.111
1100	31.502	136.376	93.504	47.159	-166.057	-119.839	23.809
1200	31.548	139.119	97.192	50.312	-165.837	-115.628	21.058
1300	31.585	141.646	100.516	53.469	-165.629	-111.446	18.736
1400	31.613	143.988	103.539	56.629	-165.436	-107.291	16.749
1500	31.636	146.170	106.309	59.791	-165.262	-103.143	15.028
1600	31.655	148.212	108.865	62.956	-165.106	-99.001	13.523
1700	31.671	150.132	111.237	66.122	-164.968	-94.867	12.196
1800	31.684	151.942	113.448	69.290	-164.849	-90.751	11.019
1900	31.696	153.656	115.520	72.459	-164.750	-86.648	9.967
2000	31.705	155.282	117.467	75.629	-164.678	-82.531	9.019

Phase changes: 478.9 K, melting point of $NbCl_5$; ΔH° = 8.097 kcal/mol.
519.7 K, boiling point of $NbCl_5$; ΔH° = 12.462 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-478.9 K: $Cp^\circ = 35.350$

$H^\circ - H^\circ_{298} = 35.350\times10^{-3}T - 10.540$

478.9-519.7 K: $Cp^\circ = 62.699 - 21.878\times10^{-3}T$

$H^\circ - H^\circ_{298} = 62.699\times10^{-3}T - 10.939\times10^{-6}T^2 - 13.032$

519.7-2000 K: $Cp^\circ = 31.771 + 0.010\times10^{-3}T - 3.360\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 31.771\times10^{-3}T + 0.005\times10^{-6}T^2 + 3.360\times10^{2}T^{-1} + 11.901$

Formation equations (kcal/mol):

298.15-478.9 K: $\Delta Hf^\circ = -192.389 + 8.087\times10^{-3}T - 0.992\times10^{-6}T^2 - 150.150T^{-1}$

$\Delta Gf^\circ = -192.389 - 8.087\times10^{-3}T\ln T + 0.992\times10^{-6}T^2 - 75.075T^{-1} + 143.489\times10^{-3}T$

478.9-519.7 K: $\Delta Hf^\circ = -194.881 + 35.436\times10^{-3}T - 11.931\times10^{-6}T^2 - 150.150T^{-1}$

$\Delta Gf^\circ = -194.881 - 35.436\times10^{-3}T\ln T + 11.931\times10^{-6}T^2 - 75.075T^{-1} + 312.237\times10^{-3}T$

519.7-2000 K: $\Delta Hf^\circ = -169.948 + 4.508\times10^{-3}T - 0.987\times10^{-6}T^2 + 185.850T^{-1}$

$\Delta Gf^\circ = -169.948 - 4.508\times10^{-3}T\ln T + 0.987\times10^{-6}T^2 + 92.925T^{-1} + 75.927\times10^{-3}T$

Source: Enthalpy of formation at 298 K from Lavut (142). Other data from Chase (26).

$NbCl_5(g)$

Niobium Pentachloride (ideal gas)

[Formation: $Nb(c) + 2.5Cl_2(g) = NbCl_5(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	28.451	96.557	96.557	0	-168.100	-154.574	113.304
300	28.485	96.733	96.557	.053	-168.096	-154.488	112.543
400	29.782	105.128	97.693	2.974	-167.850	-149.992	81.951
500	30.457	111.853	99.875	5.989	-167.582	-145.557	63.622
600	30.846	117.444	102.351	9.056	-167.311	-141.175	51.422
700	31.088	122.218	104.857	12.153	-167.042	-136.846	42.725
800	31.249	126.381	107.292	15.271	-166.783	-132.551	36.211
900	31.361	130.068	109.621	18.402	-166.529	-128.283	31.151
1000	31.442	133.377	111.835	21.542	-166.288	-124.050	27.111
1100	31.502	136.376	113.931	24.689	-166.057	-119.839	23.809
1200	31.548	139.119	115.917	27.842	-165.837	-115.628	21.058
1300	31.585	141.646	117.801	30.999	-165.629	-111.446	18.736
1400	31.613	143.988	119.589	34.159	-165.436	-107.291	16.749
1500	31.636	146.170	121.289	37.321	-165.262	-103.143	15.028
1600	31.655	148.212	122.908	40.486	-165.106	-99.001	13.523
1700	31.671	150.132	124.454	43.652	-164.968	-94.867	12.196
1800	31.684	151.942	125.931	46.820	-164.849	-90.751	11.019
1900	31.696	153.656	127.346	49.989	-164.750	-86.648	9.967
2000	31.705	155.282	128.702	53.159	-164.678	-82.531	9.019

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 31.483 + 0.194\times10^{-3}T - 2.747\times10^{5}T^{-2}$

$H°- H°_{298} = 31.483\times10^{-3}T + 0.097\times10^{-6}T^{2} + 2.747\times10^{2}T^{-1} - 10.317$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -169.696 + 4.220\times10^{-3}T - 0.895\times10^{-6}T^{2} + 124.550T^{-1}$

$\Delta Gf° = -169.696 - 4.220\times10^{-3}T\ln T + 0.895\times10^{-6}T^{2} + 62.275T^{-1} + 73.795\times10^{-3}T$

Source: Data from Chase (26).

NbF_5(c,l)

Niobium Pentafluoride

[Formation: $Nb(c) + 2.5F_2(g) = NbF_5(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	32.230	38.300	38.300	0	-433.500	-406.217	297.761
300	32.420	38.500	38.300	.060	-433.486	-406.047	295.801
350.7	39.900	44.090	38.729	1.880	-432.931	-401.450	250.173
350.7	33.550	52.274	38.729	4.750	-430.061	-401.450	250.173
400	34.890	56.774	40.674	6.440	-429.629	-397.454	217.156
500*	37.610	64.852	44.732	10.060	-428.634	-389.528	170.260

*NbF_5 boils near 500 K to mixture of polymers; ΔH° = 12 kcal/mol.

Phase change: 350.7 K, melting point of NbF_5; ΔH° = 2.870 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-350.7 K: $Cp^\circ = 35.708 + 0.212\times10^{-3}T$

$H^\circ - H^\circ_{298} = 35.708\times10^{-3}T + 0.106\times10^{-6}T^2 - 10.656$

350.7-500 K: $Cp^\circ = 24.006 + 27.170\times10^{-3}T$

$H^\circ - H^\circ_{298} = 24.006\times10^{-3}T + 13.585\times10^{-6}T^2 - 5.340$

Formation equations (kcal/mol):

298.15-350.7 K: $\Delta Hf^\circ = -435.384 + 9.242\times10^{-3}T - 1.101\times10^{-6}T^2 - 230.650T^{-1}$

$\Delta Gf^\circ = -435.384 - 9.242\times10^{-3}T\ln T + 1.101\times10^{-6}T^2 - 115.325T^{-1} + 151.453\times10^{-3}T$

350.7-500 K: $\Delta Hf^\circ = -430.068 - 2.460\times10^{-3}T + 12.378\times10^{-6}T^2 - 230.650T^{-1}$

$\Delta Gf^\circ = -430.068 + 2.460\times10^{-3}T\ln T - 12.378\times10^{-6}T^2 - 115.325T^{-1} + 72.448\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (254). Low-temperature heat capacities and entropy at 298 K from Brady (18). High-temperature data based on Brady (18) and Myers (168).

$NdBr_3(c,l)$

Neodymium Tribromide

[Formation: $Nd(c,l) + 1.5Br_2(l,g) = NdBr_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	23.700	46.400	46.400	0	-208.700	-201.166	147.457
300	23.723	46.547	46.400	.044	-208.716	-201.118	146.512
332.6	24.062	49.012	46.538	.823	-209.035	-200.276	131.599
332.6	24.062	49.012	46.538	.823	-219.633	-200.276	131.599
400	24.764	53.521	47.344	2.471	-219.325	-196.387	107.299
500	25.607	59.140	49.160	4.990	-218.834	-190.711	83.359
600	26.370	63.877	51.227	7.590	-218.312	-185.132	67.433
700	27.095	67.996	53.335	10.263	-217.767	-179.642	56.086
800	27.800	71.661	55.401	13.008	-217.206	-174.236	47.598
900	28.493	74.975	57.394	15.823	-216.642	-168.901	41.014
955	28.871	76.677	58.457	17.400	-216.331	-165.993	37.987
955	37.000	88.017	58.457	28.230	-205.501	-165.993	37.987
1000	37.000	89.720	59.825	29.895	-204.888	-164.145	35.873
1100	37.000	93.247	62.706	33.595	-203.581	-160.135	31.816
1128	37.000	94.177	63.476	34.631	-203.229	-159.039	30.813
1128	37.000	94.177	63.476	34.631	-203.953	-159.039	30.813
1200	37.000	96.466	65.387	37.295	-203.033	-156.201	28.448
1289	37.000	99.114	67.626	40.588	-201.896	-152.776	25.903
1289	37.000	99.114	67.626	40.588	-203.603	-152.776	25.903
1300	37.000	99.428	67.893	40.995	-203.461	-152.345	25.611

*Entropy and heat capacity at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
955 K, melting point of $NdBr_3$; ΔH° = 10.830 kcal/mol.
1128 K, α - β transition point of Nd; ΔH° = 0.724 kcal/mol.
1289 K, melting point of Nd; ΔH° = 1.707 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-955 K: $Cp^\circ = 22.580 + 6.676\times10^{-3}T - 0.779\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 22.580\times10^{-3}T + 3.338\times10^{-6}T^2 + 0.779\times10^{2}T^{-1} - 7.290$

955-1300 K: $Cp^\circ = 37.000$

$H^\circ - H^\circ_{298} = 37.000\times10^{-3}T - 7.105$

$NdBr_3$(c,l) - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -206.709 - 8.524\times10^{-3}T + 0.523\times10^{-6}T^2 + 150.300T^{-1}$

$\Delta Gf^\circ = -206.709 + 8.524\times10^{-3}T\ln T - 0.523\times10^{-6}T^2 + 75.150T^{-1} - 30.668\times10^{-3}T$

332.6-955 K: $\Delta Hf^\circ = -221.710 + 5.217\times10^{-3}T + 0.290\times10^{-6}T^2 + 103.200T^{-1}$

$\Delta Gf^\circ = -221.710 - 5.217\times10^{-3}T\ln T - 0.290\times10^{-6}T^2 + 51.600T^{-1} + 94.365\times10^{-3}T$

955-1128 K: $\Delta Hf^\circ = -221.525 + 19.637\times10^{-3}T - 3.048\times10^{-6}T^2 + 25.300T^{-1}$

$\Delta Gf^\circ = -221.525 - 19.637\times10^{-3}T\ln T + 3.048\times10^{-6}T^2 + 12.650T^{-1} + 189.972\times10^{-3}T$

1128-1289 K: $\Delta Hf^\circ = -218.411 + 12.947\times10^{-3}T - 0.083\times10^{-6}T^2 - 47.100T^{-1}$

$\Delta Gf^\circ = -218.411 - 12.947\times10^{-3}T\ln T + 0.083\times10^{-6}T^2 - 23.550T^{-1} + 143.566\times10^{-3}T$

1289-1300 K: $\Delta Hf^\circ = -220.296 + 13.085\times10^{-3}T - 0.083\times10^{-6}T^2 - 47.100T^{-1}$

$\Delta Gf^\circ = -220.296 - 13.085\times10^{-3}T\ln T + 0.083\times10^{-6}T^2 - 23.550T^{-1} + 146.016\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Hurtgen (103). Entropy and heat capacity at 298 K estimated. High-temperature data based on Dworkin (69).

$NdBr_3(g)$

Neodymium Tribromide (ideal gas)

[Formation: $Nd(c,l) + 1.5Br_2(l,g) = NdBr_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.132	96.024	96.024	0	-138.200	-145.462	106.625
300	19.142	96.142	96.025	.035	-138.225	-145.505	105.999
332.6	19.268	98.123	96.136	.661	-138.697	-146.272	96.114
332.6	19.268	98.123	96.136	.661	-149.294	-146.272	96.114
400	19.527	101.705	96.780	1.970	-149.326	-145.661	79.585
500	19.831	106.096	98.220	3.938	-149.386	-144.741	63.266
600	20.120	109.737	99.844	5.936	-149.465	-143.802	52.379
700	20.393	112.860	101.486	7.962	-149.568	-142.848	44.599
800	20.638	115.599	103.081	10.014	-149.701	-141.880	38.759
900	20.847	118.042	104.611	12.088	-149.877	-140.896	34.214
1000	21.017	120.248	106.066	14.182	-150.101	-139.886	30.572
1100	21.150	122.257	107.448	16.290	-150.386	-138.851	27.587
1128	21.177	122.789	107.822	16.883	-150.478	-138.562	26.846
1128	21.177	122.789	107.822	16.883	-151.202	-138.562	26.846
1200	21.248	124.102	108.759	18.411	-151.417	-137.748	25.087
1289	21.307	125.625	109.873	20.305	-151.679	-136.732	23.183
1289	21.307	125.625	109.873	20.305	-153.386	-136.732	23.183
1300	21.314	125.806	110.007	20.539	-153.417	-136.592	22.963
1400	21.352	127.387	111.193	22.672	-153.695	-135.286	21.119
1500	21.368	128.861	112.322	24.809	-153.972	-133.971	19.519
1600	21.366	130.240	113.399	26.945	-154.251	-132.627	18.116
1700	21.350	131.534	114.428	29.081	-154.533	-131.263	16.875
1800	21.322	132.754	115.412	31.215	-154.817	-129.888	15.770
1900	21.286	133.906	116.356	33.345	-155.107	-128.491	14.780
2000	21.245	134.997	117.261	35.472	-155.403	-127.084	13.887

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.
1128 K, α - β transition point of Nd; $\Delta H° = 0.724$ kcal/mol.
1289 K, melting point of Nd; $\Delta H° = 1.707$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.961 + 0.936\times10^{-3}T - 0.985\times10^{5}T^{-2}$

$H°- H°_{298} = 19.961\times10^{-3}T + 0.468\times10^{-6}T^2 + 0.985\times10^{2}T^{-1} - 6.323$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -135.242 - 11.143\times10^{-3}T - 2.347\times10^{-6}T^2 + 170.900T^{-1}$

$\Delta Gf° = -135.242 + 11.143\times10^{-3}T\ln T + 2.347\times10^{-6}T^2 + 85.450T^{-1} - 99.428\times10^{-3}T$

332.6-1128 K: $\Delta Hf° = -150.243 + 2.598\times10^{-3}T - 2.579\times10^{-6}T^2 + 123.800T^{-1}$

$\Delta Gf° = -150.243 - 2.598\times10^{-3}T\ln T + 2.579\times10^{-6}T^2 + 61.900T^{-1} + 25.604\times10^{-3}T$

1128-1289 K: $\Delta Hf° = -147.129 - 4.092\times10^{-3}T + 0.386\times10^{-6}T^2 + 51.400T^{-1}$

$\Delta Gf° = -147.129 + 4.092\times10^{-3}T\ln T - 0.386\times10^{-6}T^2 + 25.700T^{-1} - 20.802\times10^{-3}T$

1289-2000 K: $\Delta Hf° = -149.014 - 3.954\times10^{-3}T + 0.386\times10^{-6}T^2 + 51.400T^{-1}$

$\Delta Gf° = -149.014 + 3.954\times10^{-3}T\ln T - 0.386\times10^{-6}T^2 + 25.700T^{-1} - 18.352\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

$NdCl_3(c,l)$
Neodymium Trichloride
[Formation: $Nd(c,l) + 1.5Cl_2(g) = NdCl_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	23.720	36.670	36.670	0	-249.000	-231.002	169.327
300*	23.740	36.820	36.673	.044	-248.989	-230.890	168.201
400	24.800	43.790	37.615	2.470	-248.480	-224.933	122.896
500	25.900	49.440	39.432	5.004	-247.932	-219.110	95.772
600	27.000	54.250	41.507	7.646	-247.339	-213.397	77.729
700	28.000	58.490	43.639	10.396	-246.695	-207.789	64.874
800	29.100	62.300	45.733	13.254	-246.008	-202.278	55.259
900	30.200	65.800	47.779	16.219	-245.280	-196.864	47.804
1000	31.300	69.030	49.737	19.293	-244.514	-191.517	41.856
1032	31.600	70.020	50.351	20.300	-244.262	-189.825	40.199
1032	35.000	81.650	50.351	32.300	-232.262	-189.825	40.199
1100	35.000	83.890	52.363	34.680	-231.513	-187.063	37.165
1128	35.000	84.770	53.156	35.660	-231.216	-185.940	36.025
1128	35.000	84.770	53.156	35.660	-231.940	-185.940	36.025
1200	35.000	86.930	55.113	38.180	-231.160	-183.023	33.333
1289	35.000	89.433	57.396	41.295	-230.197	-179.492	30.432
1289	35.000	89.433	57.396	41.295	-231.904	-179.492	30.432
1300	35.000	89.730	57.668	41.680	-231.784	-179.047	30.100

*Data 300-1000 K estimated.

Phase changes: 1032 K, melting point of $NdCl_3$; $\Delta H°$ = 12.000 kcal/mol.
1128 K, α - β transition point of Nd; $\Delta H°$ = 0.724 kcal/mol.
1289 K, melting point of Nd; $\Delta H°$ = 1.707 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1032 K: $Cp° = 20.466 + 10.814\times10^{-3}T + 0.014\times10^{5}T^{-2}$
$H°- H°_{298} = 20.466\times10^{-3}T + 5.407\times10^{-6}T^2 - 0.014\times10^{2}T^{-1} - 6.578$

1032-1300 K: $Cp° = 35.000$
$H°- H°_{298} = 35.000\times10^{-3}T - 3.820$

Formation equations (kcal/mol):

298.15-1032 K: $\Delta Hf° = -250.071 + 3.257\times10^{-3}T + 2.310\times10^{-6}T^2 - 31.450T^{-1}$
$\Delta Gf° = -250.071 - 3.257\times10^{-3}T\ln T - 2.310\times10^{-6}T^2 - 15.725T^{-1} + 83.383\times10^{-3}T$

1032-1128 K: $\Delta Hf° = -247.313 + 17.792\times10^{-3}T - 3.097\times10^{-6}T^2 - 30.050T^{-1}$
$\Delta Gf° = -247.313 - 17.792\times10^{-3}T\ln T + 3.097\times10^{-6}T^2 - 15.025T^{-1} + 175.985\times10^{-3}T$

1128-1289 K: $\Delta Hf° = -244.199 + 11.102\times10^{-3}T - 0.132\times10^{-6}T^2 - 102.450T^{-1}$
$\Delta Gf° = -244.199 - 11.102\times10^{-3}T\ln T + 0.132\times10^{-6}T^2 - 51.225T^{-1} + 129.579\times10^{-3}T$

1289-1300 K: $\Delta Hf° = -246.084 + 11.240\times10^{-3}T - 0.132\times10^{-6}T^2 - 102.450T^{-1}$
$\Delta Gf° = -246.084 - 11.240\times10^{-3}T\ln T + 0.132\times10^{-6}T^2 - 51.225T^{-1} + 132.029\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Stuve (231). Low-temperature heat capacities and entropy at 298 K from Sommers (219). High-temperature data between 298 K and 1032 K estimated. Values at 1032 K, enthalpy of fusion, and heat capacity of liquid based on Dworkin (66).

$NdCl_3(g)$

Neodymium Trichloride (ideal gas)

[Formation: $Nd(c,l) + 1.5Cl_2(g) = NdCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.721	89.453	89.453	0	-171.800	-169.539	124.274
300	18.734	89.569	89.453	.035	-171.798	-169.524	123.497
400	19.278	95.039	90.194	1.938	-171.813	-168.765	92.208
500	19.666	99.384	91.614	3.885	-171.851	-168.001	73.432
600	20.003	103.000	93.218	5.869	-171.915	-167.224	60.910
700	20.306	106.107	94.843	7.885	-172.006	-166.432	51.962
800	20.570	108.836	96.425	9.929	-172.133	-165.632	45.248
900	20.793	111.272	97.941	11.998	-172.301	-164.809	40.021
1000	20.974	113.472	99.386	14.086	-172.521	-163.966	35.834
1100	21.114	115.478	100.759	16.191	-172.802	-163.098	32.404
1128	21.143	116.009	101.131	16.783	-172.893	-162.856	31.553
1128	21.143	116.009	101.131	16.783	-173.617	-162.856	31.553
1200	21.217	117.320	102.063	18.308	-173.832	-162.163	29.534
1289	21.280	118.840	103.170	20.199	-174.093	-161.294	27.347
1289	21.280	118.840	103.170	20.199	-175.800	-161.294	27.347
1300	21.288	119.021	103.303	20.433	-175.831	-161.172	27.095
1400	21.330	120.601	104.484	22.564	-176.108	-160.035	24.982
1500	21.349	122.073	105.607	24.699	-176.384	-158.884	23.149
1600	21.349	123.451	106.680	26.834	-176.663	-157.707	21.541
1700	21.334	124.745	107.705	28.968	-176.945	-156.508	20.120
1800	21.308	125.964	108.686	31.100	-177.231	-155.302	18.856
1900	21.274	127.115	109.626	33.229	-177.522	-154.071	17.722
2000	21.234	128.205	110.528	35.355	-177.821	-152.829	16.700

Phase changes: 1128 K, α - β transition point of Nd; $\Delta H°$ = 0.724 kcal/mol.
1289 K, melting point of Nd; $\Delta H°$ = 1.707 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.930 + 0.954\times10^{-3}T - 1.327\times10^{5}T^{-2}$

$H°- H°_{298} = 19.930\times10^{-3}T + 0.477\times10^{-6}T^2 + 1.327\times10^{2}T^{-1} - 6.430$

Formation equations (kcal/mol):

298.15-1128 K: $\Delta Hf° = -172.723 + 2.721\times10^{-3}T - 2.620\times10^{-6}T^2 + 102.650T^{-1}$

$\Delta Gf° = -172.723 - 2.721\times10^{-3}T\ln T + 2.620\times10^{-6}T^2 + 51.325T^{-1} + 24.825\times10^{-3}T$

1128-1289 K: $\Delta Hf° = -169.609 - 3.968\times10^{-3}T + 0.345\times10^{-6}T^2 + 30.250T^{-1}$

$\Delta Gf° = -169.609 + 3.968\times10^{-3}T\ln T - 0.345\times10^{-6}T^2 + 15.125T^{-1} - 21.582\times10^{-3}T$

1289-2000 K: $\Delta Hf° = -171.494 - 3.830\times10^{-3}T + 0.345\times10^{-6}T^2 + 30.250T^{-1}$

$\Delta Gf° = -171.494 + 3.830\times10^{-3}T\ln T - 0.345\times10^{-6}T^2 + 15.125T^{-1} - 19.131\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

NdF_3(c,l)

Neodymium Trifluoride

[Formation: $Nd(c,l) + 1.5F_2(g) = NdF_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	22.090	28.870	28.870	0	-401.400	-383.244	280.922
300	22.125	29.007	28.870	.041	-401.391	-383.131	279.107
400	23.554	35.595	29.760	2.334	-400.923	-377.113	206.043
500	24.418	40.949	31.479	4.735	-400.435	-371.219	162.258
600	25.094	45.462	33.442	7.212	-399.947	-365.420	133.103
700	25.697	49.376	35.445	9.752	-399.468	-359.700	112.302
800	26.275	52.846	37.409	12.350	-399.005	-354.056	96.722
900	26.850	55.973	39.299	15.007	-398.557	-348.463	84.617
1000	27.434	58.833	41.112	17.721	-398.131	-342.921	74.944
1100	28.034	61.475	42.844	20.494	-397.727	-337.420	67.038
1128	28.208	62.182	43.315	21.281	-397.618	-335.891	65.078
1128	28.208	62.182	43.315	21.281	-398.342	-335.891	65.078
1200	28.655	63.941	44.501	23.328	-398.026	-331.917	60.450
1289	29.228	66.011	45.915	25.904	-397.593	-327.033	55.448
1289	29.228	66.011	45.915	25.904	-399.300	-327.033	55.448
1300	29.299	66.260	46.086	26.226	-399.242	-326.419	54.875
1400	29.967	68.455	47.606	29.189	-398.681	-320.838	50.084
1500	30.661	70.546	49.066	32.220	-398.056	-315.308	45.940
1600	31.381	72.548	50.472	35.322	-397.366	-309.812	42.318
1650	31.752	73.520	51.156	36.900	-396.993	-307.077	40.673
1650	41.300	81.459	51.156	50.000	-383.893	-307.077	40.673
1700	41.300	82.692	52.066	52.065	-383.036	-304.763	39.179
1800	41.300	85.052	53.833	56.195	-381.326	-300.209	36.450

Phase changes: 1128 K, α - β transition point of Nd; $\Delta H° = 0.724$ kcal/mol.
1289 K, melting point of Nd; $\Delta H° = 1.707$ kcal/mol.
1650 K, melting point of NdF_3; $\Delta H° = 13.100$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1650 K: $Cp° = 22.155 + 5.600\times10^{-3}T - 1.543\times10^{5}T^{-2}$

$H°- H°_{298} = 22.155\times10^{-3}T + 2.800\times10^{-6}T^{2} + 1.543\times10^{2}T^{-1} - 7.372$

1650-1800 K: $Cp° = 41.300$

$H°- H°_{298} = 41.300\times10^{-3}T - 18.145$

NdF_3(c,1) - Continued

Formation equations (kcal/mol):

298.15-1128 K: $\Delta Hf^\circ = -403.234 + 5.425\times10^{-3}T - 0.426\times10^{-6}T^2 + 75.950T^{-1}$

$\Delta Gf^\circ = -403.234 - 5.425\times10^{-3}T\ln T + 0.426\times10^{-6}T^2 + 37.975T^{-1} + 97.402\times10^{-3}T$

1128-1289 K: $\Delta Hf^\circ = -400.120 - 1.265\times10^{-3}T + 2.539\times10^{-6}T^2 + 3.550T^{-1}$

$\Delta Gf^\circ = -400.120 + 1.265\times10^{-3}T\ln T - 2.539\times10^{-6}T^2 + 1.775T^{-1} + 50.996\times10^{-3}T$

1289-1650 K: $\Delta Hf^\circ = -402.005 - 1.127\times10^{-3}T + 2.539\times10^{-6}T^2 + 3.550T^{-1}$

$\Delta Gf^\circ = -402.005 + 1.127\times10^{-3}T\ln T - 2.539\times10^{-6}T^2 + 1.775T^{-1} + 53.446\times10^{-3}T$

1650-1800 K: $\Delta Hf^\circ = -412.778 + 18.018\times10^{-3}T - 0.261\times10^{-6}T^2 - 150.750T^{-1}$

$\Delta Gf^\circ = -412.778 - 18.018\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 - 75.375T^{-1} + 197.220\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Johnson (111). Low-temperature heat capacities and entropy at 298 K from Lyon (146). High-temperature data based on Spedding (223) and Charlu (23).

$NdF_3(g)$

Neodymium Trifluoride (ideal gas)

[Formation: $Nd(c,l) + 1.5F_2(g) = NdF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	17.256	81.419	81.419	0	-296.100	-293.612	215.220
300	17.280	81.526	81.419	.032	-296.100	-293.596	213.882
400	18.302	86.649	82.112	1.815	-296.143	-292.754	159.951
500	18.985	90.810	83.448	3.681	-296.189	-291.904	127.589
600	19.508	94.320	84.975	5.607	-296.253	-291.040	106.010
700	19.931	97.360	86.531	7.580	-296.341	-290.161	90.591
800	20.278	100.045	88.056	9.591	-296.465	-289.274	79.025
900	20.559	102.450	89.524	11.633	-296.631	-288.366	70.024
1000	20.783	104.628	90.927	13.701	-296.851	-287.437	62.818
1100	20.955	106.617	92.264	15.788	-297.133	-286.482	56.918
1128	20.991	107.144	92.627	16.375	-297.224	-286.215	55.453
1128	20.991	107.144	92.627	16.375	-297.948	-286.215	55.453
1200	21.083	108.446	93.538	17.890	-298.165	-285.461	51.989
1289	21.163	109.958	94.621	19.770	-298.427	-284.514	48.239
1289	21.163	109.958	94.621	19.770	-300.134	-284.514	48.239
1300	21.173	110.138	94.751	20.003	-300.165	-284.383	47.809
1400	21.230	111.709	95.906	22.124	-300.446	-283.159	44.203
1500	21.262	113.175	97.010	24.248	-300.729	-281.924	41.076
1600	21.272	114.548	98.064	26.375	-301.013	-280.659	38.336
1700	21.266	115.837	99.071	28.502	-301.299	-279.372	35.915
1800	21.248	117.052	100.036	30.628	-301.594	-278.077	33.763
1900	21.219	118.200	100.962	32.752	-301.891	-276.758	31.834
2000	21.184	119.288	101.852	34.872	-302.198	-275.428	30.097

Phase changes: 1128 K, α - β transition point of Nd; ΔH° = 0.724 kcal/mol.
1289 K, melting point of Nd; ΔH° = 1.707 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.649 + 1.114\times10^{-3}T - 2.423\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.649\times10^{-3}T + 0.557\times10^{-6}T^2 + 2.423\times10^{2}T^{-1} - 6.721$

Formation equations (kcal/mol):

298.15-1128 K: $\Delta Hf^\circ = -297.283 + 2.919\times10^{-3}T - 2.669\times10^{-6}T^2 + 163.950T^{-1}$

$\Delta Gf^\circ = -297.283 - 2.919\times10^{-3}T\ln T + 2.669\times10^{-6}T^2 + 81.975T^{-1} + 27.227\times10^{-3}T$

1128-1289 K: $\Delta Hf^\circ = -294.169 - 3.771\times10^{-3}T + 0.296\times10^{-6}T^2 + 91.550T^{-1}$

$\Delta Gf^\circ = -294.169 + 3.771\times10^{-3}T\ln T - 0.296\times10^{-6}T^2 + 45.775T^{-1} - 19.180\times10^{-3}T$

1289-2000 K: $\Delta Hf^\circ = -296.054 - 3.633\times10^{-3}T + 0.296\times10^{-6}T^2 + 91.550T^{-1}$

$\Delta Gf^\circ = -296.054 + 3.633\times10^{-3}T\ln T - 0.296\times10^{-6}T^2 + 45.775T^{-1} - 16.729\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

$NdI_3(c,l)$

Neodymium Triiodide

[Formation: $Nd(c,l) + 1.5I_2(c,l,g) = NdI_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	23.600	55.100	55.100	0	-152.800	-151.716	111.209
300	23.632	55.246	55.100	.044	-152.803	-151.707	110.517
386.8	24.826	61.411	55.850	2.151	-153.089	-151.358	85.519
386.8	24.826	61.411	55.850	2.151	-158.653	-151.358	85.519
400	25.008	62.247	56.047	2.480	-158.797	-151.107	82.560
458.4	25.607	65.698	57.060	3.960	-159.413	-149.939	71.485
458.4	25.607	65.698	57.060	3.960	-174.444	-149.939	71.485
500	26.033	67.941	57.873	5.034	-174.226	-147.722	64.568
600	26.921	72.767	59.962	7.683	-173.668	-142.471	51.895
700	27.744	76.980	62.100	10.416	-173.072	-137.316	42.872
800	28.533	80.736	64.199	13.230	-172.452	-132.252	36.129
847	28.897	82.375	65.162	14.580	-172.154	-129.898	33.517
847	27.980	86.307	65.162	17.910	-168.824	-129.898	33.517
900	27.980	88.005	66.457	19.393	-168.547	-127.474	30.954
1000	27.980	90.953	68.762	22.191	-168.074	-122.935	26.867
1060	27.980	92.584	70.065	23.870	-167.826	-120.235	24.790
1060	37.200	101.942	70.065	33.790	-157.906	-120.235	24.790
1100	37.200	103.320	71.249	35.278	-157.388	-118.823	23.608
1128	37.200	104.255	72.057	36.320	-157.032	-117.851	22.833
1128	37.200	104.255	72.057	36.320	-157.756	-117.851	22.833
1200	37.200	106.557	74.059	38.998	-156.828	-115.334	21.005
1289	37.200	109.219	76.396	42.309	-155.678	-112.304	19.041
1289	37.200	109.219	76.396	42.309	-157.385	-112.304	19.041
1300	37.200	109.535	76.675	42.718	-157.243	-111.922	18.816

*Entropy and heat capacity at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
847 K, α - β transition point of NdI_3; ΔH° = 3.330 kcal/mol.
1060 K, melting point of NdI_3; ΔH° = 9.920 kcal/mol.
1128 K, α - β transition point of Nd; ΔH° = 0.724 kcal/mol.
1289 K, melting point of Nd; ΔH° = 1.707 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-847 K: $Cp^\circ = 22.945 + 7.248\times10^{-3}T - 1.338\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 22.945\times10^{-3}T + 3.624\times10^{-6}T^2 + 1.338\times10^{2}T^{-1} - 7.612$

847-1060 K: $Cp^\circ = 27.980$

$H^\circ - H^\circ_{298} = 27.980\times10^{-3}T - 5.789$

1060-1300 K: $Cp^\circ = 37.200$

$H^\circ - H^\circ_{298} = 37.200\times10^{-3}T - 5.642$

NdI_3(c,1) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -153.250 - 0.339\times10^{-3}T - 1.579\times10^{-6}T^2 + 206.200T^{-1}$

$\Delta Gf^\circ = -153.250 + 0.339\times10^{-3}T\ln T + 1.579\times10^{-6}T^2 + 103.100T^{-1} + 1.588\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -155.433 - 9.944\times10^{-3}T + 0.659\times10^{-6}T^2 + 206.200T^{-1}$

$\Delta Gf^\circ = -155.433 + 9.944\times10^{-3}T\ln T - 0.659\times10^{-6}T^2 + 103.100T^{-1} - 49.135\times10^{-3}T$

458.4-847 K: $\Delta Hf^\circ = -177.503 + 5.565\times10^{-3}T + 0.557\times10^{-6}T^2 + 183.250T^{-1}$

$\Delta Gf^\circ = -177.503 - 5.565\times10^{-3}T\ln T - 0.557\times10^{-6}T^2 + 91.625T^{-1} + 94.060\times10^{-3}T$

847-1060 K: $\Delta Hf^\circ = -175.680 + 10.601\times10^{-3}T - 3.067\times10^{-6}T^2 + 49.450T^{-1}$

$\Delta Gf^\circ = -175.680 - 10.601\times10^{-3}T\ln T + 3.067\times10^{-6}T^2 + 24.725T^{-1} + 122.875\times10^{-3}T$

1060-1128 K: $\Delta Hf^\circ = -175.533 + 19.820\times10^{-3}T - 3.067\times10^{-6}T^2 + 49.450T^{-1}$

$\Delta Gf^\circ = -175.533 - 19.820\times10^{-3}T\ln T + 3.067\times10^{-6}T^2 + 24.725T^{-1} + 186.964\times10^{-3}T$

1128-1289 K: $\Delta Hf^\circ = -172.419 + 13.131\times10^{-3}T - 0.102\times10^{-6}T^2 - 22.950T^{-1}$

$\Delta Gf^\circ = -172.419 - 13.131\times10^{-3}T\ln T + 0.102\times10^{-6}T^2 - 11.475T^{-1} + 140.557\times10^{-3}T$

1289-1300 K: $\Delta Hf^\circ = -174.304 + 13.269\times10^{-3}T - 0.102\times10^{-6}T^2 - 22.950T^{-1}$

$\Delta Gf^\circ = -174.304 - 13.269\times10^{-3}T\ln T + 0.102\times10^{-6}T^2 - 11.475T^{-1} + 143.008\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (207). Entropy and heat capacity at 298 K estimated. High-temperature data based on Dworkin (69).

$NdI_3(g)$

Neodymium Triiodide (ideal gas)

[Formation: $Nd(c,l) + 1.5I_2(c,l,g) = NdI_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.498	102.900	102.900	0	-87.600	-100.767	73.863
300	19.503	103.021	102.901	.036	-87.611	-100.848	73.467
386.8	19.709	108.003	103.508	1.739	-88.302	-104.592	59.096
386.8	19.709	108.003	103.508	1.739	-93.865	-104.592	59.096
400	19.740	108.665	103.668	1.999	-94.078	-104.955	57.344
458.4	19.874	111.364	104.481	3.155	-95.017	-106.477	50.764
458.4	19.874	111.364	104.481	3.155	-110.049	-106.477	50.764
500	19.970	113.095	105.127	3.984	-110.076	-106.149	46.397
600	20.218	116.757	106.769	5.993	-110.158	-105.355	38.375
700	20.466	119.893	108.424	8.028	-110.260	-104.543	32.640
800	20.693	122.641	110.034	10.086	-110.396	-103.720	28.335
900	20.891	125.090	111.573	12.165	-110.575	-102.878	24.982
1000	21.053	127.300	113.037	14.263	-110.802	-102.010	22.294
1100	21.180	129.312	114.426	16.375	-111.090	-101.117	20.090
1128	21.206	129.845	114.802	16.968	-111.183	-100.868	19.543
1128	21.206	129.845	114.802	16.968	-111.907	-100.868	19.543
1200	21.273	131.160	115.745	18.498	-112.128	-100.158	18.241
1289	21.328	132.684	116.863	20.393	-112.394	-99.266	16.830
1289	21.328	132.684	116.863	20.393	-114.101	-99.266	16.830
1300	21.335	132.865	116.997	20.628	-114.132	-99.141	16.667
1400	21.371	134.448	118.188	22.764	-114.417	-97.976	15.295
1500	21.384	135.922	119.321	24.902	-114.700	-96.801	14.104
1600	21.380	137.303	120.403	27.040	-114.985	-95.596	13.058
1700	21.362	138.598	121.435	29.177	-115.274	-94.372	12.132
1800	21.333	139.819	122.423	31.312	-115.567	-93.138	11.308
1900	21.296	140.971	123.369	33.444	-115.865	-91.879	10.568
2000	21.254	142.062	124.276	35.571	-116.170	-90.608	9.901

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
1128 K, α - β transition point of Nd; $\Delta H°$ = 0.724 kcal/mol.
1289 K, melting point of Nd; $\Delta H°$ = 1.707 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.980 + 0.926\times10^{-3}T - 0.674\times10^{5}T^{-2}$

$H°- H°_{298} = 19.980\times10^{-3}T + 0.463\times10^{-6}T^2 + 0.674\times10^{2}T^{-1} - 6.224$

$NdI_3(g)$ - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -86.663 - 3.303\times10^{-3}T - 4.740\times10^{-6}T^2 + 139.800T^{-1}$

$\Delta Gf^\circ = -86.663 + 3.303\times10^{-3}T\ln T + 4.740\times10^{-6}T^2 + 69.900T^{-1} - 68.329\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -88.845 - 12.910\times10^{-3}T - 2.502\times10^{-6}T^2 + 139.800T^{-1}$

$\Delta Gf^\circ = -88.845 + 12.910\times10^{-3}T\ln T + 2.502\times10^{-6}T^2 + 69.900T^{-1} - 119.052\times10^{-3}T$

458.4-1128 K: $\Delta Hf^\circ = -110.915 + 2.601\times10^{-3}T - 2.604\times10^{-6}T^2 + 116.850T^{-1}$

$\Delta Gf^\circ = -110.915 - 2.601\times10^{-3}T\ln T + 2.604\times10^{-6}T^2 + 58.425T^{-1} + 24.143\times10^{-3}T$

1128-1289 K: $\Delta Hf^\circ = -107.801 - 4.089\times10^{-3}T + 0.361\times10^{-6}T^2 + 44.450T^{-1}$

$\Delta Gf^\circ = -107.801 + 4.089\times10^{-3}T\ln T - 0.361\times10^{-6}T^2 + 22.225T^{-1} - 22.263\times10^{-3}T$

1289-2000 K: $\Delta Hf^\circ = -109.686 - 3.951\times10^{-3}T + 0.361\times10^{-6}T^2 + 44.450T^{-1}$

$\Delta Gf^\circ = -109.686 + 3.951\times10^{-3}T\ln T - 0.361\times10^{-6}T^2 + 22.225T^{-1} - 19.813\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

NiBr(g)

Nickel Monobromide (ideal gas)

[Formation: $Ni(c,l) + 0.5Br_2(l,g) = NiBr(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.645	62.709	62.709	0	44.000	32.855	-24.083
300	8.651	62.762	62.709	.016	43.987	32.787	-23.885
332.6	8.744	63.659	62.759	.300	43.771	31.580	-20.751
332.6	8.744	63.659	62.759	.300	40.239	31.580	-20.751
400	8.936	65.291	63.051	.896	40.095	29.838	-16.302
500	9.172	67.312	63.708	1.802	39.850	27.300	-11.932
600	9.356	69.001	64.453	2.729	39.550	24.815	-9.039
631	9.396	69.473	64.688	3.020	39.434	24.059	-8.333
700	9.485	70.454	65.210	3.671	39.248	22.389	-6.990
800	9.567	71.726	65.946	4.624	39.017	19.994	-5.462
900	9.612	72.856	66.653	5.583	38.778	17.629	-4.281
1000	9.634	73.870	67.324	6.546	38.529	15.290	-3.342
1100	9.642	74.788	67.961	7.510	38.264	12.989	-2.581
1200	9.644	75.627	68.565	8.474	37.980	10.701	-1.949
1300	9.645	76.399	69.139	9.438	37.677	8.436	-1.418
1400	9.651	77.114	69.683	10.403	37.354	6.201	-.968
1500	9.664	77.781	70.202	11.369	37.009	3.985	-.581
1600	9.686	78.405	70.695	12.336	36.642	1.799	-.246
1700	9.718	78.993	71.166	13.306	36.255	-.379	.049
1728	9.730	79.152	71.294	13.578	36.142	-.966	.122
1728	9.730	79.152	71.294	13.578	32.042	-.966	.122
1800	9.761	79.550	71.617	14.280	31.746	-2.338	.284
1900	9.814	80.079	72.048	15.259	31.339	-4.224	.486
2000	9.876	80.584	72.463	16.243	30.936	-6.081	.664

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
1728 K, melting point of Ni; ΔH° = 4.100 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 9.439 + 0.202\times10^{-3}T - 0.759\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 9.439\times10^{-3}T + 0.101\times10^{-6}T^2 + 0.759\times10^{2}T^{-1} - 3.078$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = 44.691 - 2.602\times10^{-3}T - 4.129\times10^{-6}T^2 + 134.900T^{-1}$

$\Delta Gf^\circ = 44.691 + 2.602\times10^{-3}T\ln T + 4.129\times10^{-6}T^2 + 67.450T^{-1} - 56.513\times10^{-3}T$

332.6-631 K: $\Delta Hf^\circ = 39.690 + 1.978\times10^{-3}T - 4.207\times10^{-6}T^2 + 119.200T^{-1}$

$\Delta Gf^\circ = 39.690 - 1.978\times10^{-3}T\ln T + 4.207\times10^{-6}T^2 + 59.600T^{-1} - 14.836\times10^{-3}T$

631-750 K: $\Delta Hf^\circ = 42.239 - 6.346\times10^{-3}T + 2.819\times10^{-6}T^2 + 60.200T^{-1}$

$\Delta Gf^\circ = 42.239 + 6.346\times10^{-3}T\ln T - 2.819\times10^{-6}T^2 + 30.100T^{-1} - 68.036\times10^{-3}T$

750-1728 K: $\Delta Hf^\circ = 39.329 - 0.097\times10^{-3}T - 1.084\times10^{-6}T^2 + 373.800T^{-1}$

$\Delta Gf^\circ = 39.329 + 0.097\times10^{-3}T\ln T + 1.084\times10^{-6}T^2 + 186.900T^{-1} - 25.992\times10^{-3}T$

1728-2000 K: $\Delta Hf^\circ = 39.264 - 4.326\times10^{-3}T + 0.073\times10^{-6}T^2 + 60.200T^{-1}$

$\Delta Gf^\circ = 39.264 + 4.326\times10^{-3}T\ln T - 0.073\times10^{-6}T^2 + 30.100T^{-1} - 55.428\times10^{-3}T$

Source: Data from Mah (150).

$NiBr_2(c)$
Nickel Dibromide
[Formation: $Ni(c) + Br_2(l,g) = NiBr_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.020	29.260	29.260	0	-50.640	-46.389	34.003
300	18.030	29.370	29.260	.033	-50.652	-46.362	33.774
332.6	18.222	31.240	29.364	.624	-50.855	-45.885	30.151
332.6	18.222	31.240	29.364	.624	-57.920	-45.885	30.151
400	18.620	34.650	29.980	1.868	-57.711	-43.472	23.752
500	18.930	38.840	31.348	3.746	-57.425	-39.948	17.461
600	19.190	42.310	32.890	5.652	-57.189	-36.475	13.286
631	19.283	43.279	33.377	6.248	-57.138	-35.404	12.262
700	19.490	45.290	34.453	7.586	-56.946	-33.034	10.314
800	19.870	47.920	35.979	9.553	-56.611	-29.646	8.099
900	20.350	50.280	37.430	11.565	-56.246	-26.290	6.384
1000	20.930	52.460	38.835	13.625	-55.848	-22.996	5.026
1100	21.620	54.480	40.162	15.750	-55.403	-19.717	3.917
1200	22.420	56.400	41.438	17.955	-54.897	-16.499	3.005

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.
631 K, Curie temperature of Ni; $\Delta H° = 0$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 17.284 + 3.496\times10^{-3}T - 0.272\times10^{5}T^{-2}$

$H°- H°_{298} = 17.284\times10^{-3}T + 1.748\times10^{-6}T^{2} + 0.272\times10^{2}T^{-1} - 5.400$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -49.579 - 3.803\times10^{-3}T - 2.432\times10^{-6}T^{2} + 86.200T^{-1}$

$\Delta Gf° = -49.579 + 3.803\times10^{-3}T\ln T + 2.432\times10^{-6}T^{2} + 43.100T^{-1} - 12.177\times10^{-3}T$

332.6-631 K: $\Delta Hf° = -59.579 + 5.358\times10^{-3}T - 2.587\times10^{-6}T^{2} + 54.800T^{-1}$

$\Delta Gf° = -59.579 - 5.358\times10^{-3}T\ln T + 2.587\times10^{-6}T^{2} + 27.400T^{-1} + 71.178\times10^{-3}T$

631-750 K: $\Delta Hf° = -57.031 - 2.966\times10^{-3}T + 4.438\times10^{-6}T^{2} - 4.200T^{-1}$

$\Delta Gf° = -57.031 + 2.966\times10^{-3}T\ln T - 4.438\times10^{-6}T^{2} - 2.100T^{-1} + 17.978\times10^{-3}T$

750-1200 K: $\Delta Hf° = -59.941 + 3.283\times10^{-3}T + 0.536\times10^{-6}T^{2} + 309.400T^{-1}$

$\Delta Gf° = -59.941 - 3.283\times10^{-3}T\ln T - 0.536\times10^{-6}T^{2} + 154.700T^{-1} + 60.021\times10^{-3}T$

Source: Data from Stuve (232).

$NiBr_2(g)$
Nickel Dibromide (ideal gas)
[Formation: $Ni(c,l) + Br_2(l,g) = NiBr_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	15.012	76.710	76.710	0	2.800	-7.096	5.201
300	15.025	76.803	76.710	.028	2.783	-7.157	5.214
332.6	15.195	78.362	76.797	.521	2.482	-8.221	5.402
332.6	15.195	78.362	76.797	.521	-4.583	-8.221	5.402
400	15.546	81.205	77.308	1.559	-4.580	-8.963	4.897
500	15.820	84.706	78.448	3.129	-4.602	-10.058	4.396
600	15.957	87.604	79.739	4.719	-4.682	-11.144	4.059
631	15.976	88.408	80.145	5.214	-4.732	-11.475	3.974
700	16.019	90.069	81.043	6.318	-4.774	-12.207	3.811
800	16.041	92.210	82.309	7.921	-4.803	-13.270	3.625
900	16.047	94.100	83.517	9.525	-4.846	-14.328	3.479
1000	16.048	95.791	84.661	11.130	-4.903	-15.382	3.362
1100	16.050	97.320	85.743	12.735	-4.978	-16.416	3.261
1200	16.054	98.717	86.767	14.340	-5.072	-17.455	3.179
1300	16.060	100.002	87.736	15.946	-5.186	-18.485	3.108
1400	16.066	101.193	88.656	17.552	-5.321	-19.502	3.044
1500	16.071	102.301	89.528	19.159	-5.479	-20.511	2.988
1600	16.075	103.339	90.360	20.766	-5.661	-21.504	2.937
1700	16.076	104.313	91.152	22.374	-5.865	-22.500	2.892
1728	16.076	104.576	91.367	22.824	-5.927	-22.758	2.878
1728	16.076	104.576	91.367	22.824	-10.027	-22.758	2.878
1800	16.075	105.232	91.909	23.981	-10.196	-23.287	2.827
1900	16.071	106.101	92.633	25.589	-10.430	-24.011	2.762
2000	16.066	106.925	93.327	27.196	-10.667	-24.715	2.701

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
1728 K, melting point of Ni; ΔH° = 4.100 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 16.150 - 0.930\times10^5 T^{-2}$
$H^\circ - H^\circ_{298} = 16.150\times10^{-3} T + 0.930\times10^2 T^{-1} - 5.127$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = 4.134 - 4.937\times10^{-3} T - 4.180\times10^{-6} T^2 + 152.000 T^{-1}$
$\Delta Gf^\circ = 4.134 + 4.937\times10^{-3} T\ln T + 4.180\times10^{-6} T^2 + 76.000 T^{-1} - 67.895\times10^{-3} T$

332.6-631 K: $\Delta Hf^\circ = -5.867 + 4.224\times10^{-3} T - 4.335\times10^{-6} T^2 + 120.600 T^{-1}$
$\Delta Gf^\circ = -5.867 - 4.224\times10^{-3} T\ln T + 4.335\times10^{-6} T^2 + 60.300 T^{-1} + 15.460\times10^{-3} T$

631-750 K: $\Delta Hf^\circ = -3.318 - 4.100\times10^{-3} T + 2.690\times10^{-6} T^2 + 61.600 T^{-1}$
$\Delta Gf^\circ = -3.318 + 4.100\times10^{-3} T\ln T - 2.690\times10^{-6} T^2 + 30.800 T^{-1} - 37.739\times10^{-3} T$

750-1728 K: $\Delta Hf^\circ = -6.228 + 2.149\times10^{-3} T - 1.212\times10^{-6} T^2 + 375.200 T^{-1}$
$\Delta Gf^\circ = -6.228 - 2.149\times10^{-3} T\ln T + 1.212\times10^{-6} T^2 + 187.600 T^{-1} + 4.304\times10^{-3} T$

1728-2000 K: $\Delta Hf^\circ = -6.293 - 2.080\times10^{-3} T - 0.055\times10^{-6} T^2 + 61.600 T^{-1}$
$\Delta Gf^\circ = -6.293 + 2.080\times10^{-3} T\ln T + 0.055\times10^{-6} T^2 + 30.800 T^{-1} - 25.132\times10^{-3} T$

Source: Data from Mah (150).

NiCl(g)

Nickel Monochloride (ideal gas)

[Formation: $Ni(c,l) + 0.5Cl_2(g) = NiCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.446	60.061	60.061	0	43.000	35.166	-25.777
300	8.454	60.113	60.061	.016	42.996	35.118	-25.583
400	8.800	62.595	60.398	.879	42.793	32.520	-17.768
500	9.071	64.589	61.043	1.773	42.550	29.978	-13.103
600	9.275	66.262	61.777	2.691	42.252	27.488	-10.012
631	9.318	66.730	62.009	2.979	42.135	26.730	-9.258
700	9.415	67.703	62.523	3.626	41.950	25.059	-7.824
800	9.502	68.966	63.251	4.572	41.715	22.658	-6.190
900	9.551	70.089	63.950	5.525	41.476	20.289	-4.927
1000	9.575	71.096	64.614	6.482	41.223	17.946	-3.922
1100	9.583	72.009	65.245	7.440	40.955	15.641	-3.108
1200	9.584	72.843	65.845	8.398	40.667	13.349	-2.431
1300	9.586	73.611	66.414	9.356	40.359	11.080	-1.863
1400	9.592	74.321	66.953	10.315	40.031	8.843	-1.380
1500	9.607	74.983	67.466	11.275	39.681	6.626	-.965
1600	9.632	75.604	67.956	12.237	39.309	4.438	-.606
1700	9.669	76.189	68.423	13.202	38.917	2.260	-.290
1728	9.683	76.347	68.550	13.473	38.804	1.672	-.211
1728	9.683	76.347	68.550	13.473	34.704	1.672	-.211
1800	9.718	76.743	68.870	14.171	34.404	.299	-.036
1900	9.779	77.270	69.298	15.146	33.993	-1.589	.183
2000	9.850	77.773	69.710	16.127	33.587	-3.446	.377

Phase changes: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
1728 K, melting point of Ni; ΔH° = 4.100 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 9.393 + 0.202\times10^{-3}T - 0.895\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 9.393\times10^{-3}T + 0.101\times10^{-6}T^2 + 0.895\times10^{2}T^{-1} - 3.110$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf^\circ = 42.400 + 1.984\times10^{-3}T - 4.223\times10^{-6}T^2 + 114.350T^{-1}$

$\Delta Gf^\circ = 42.400 - 1.984\times10^{-3}T\ln T + 4.223\times10^{-6}T^2 + 57.175T^{-1} - 14.866\times10^{-3}T$

631-750 K: $\Delta Hf^\circ = 44.949 - 6.340\times10^{-3}T + 2.802\times10^{-6}T^2 + 55.350T^{-1}$

$\Delta Gf^\circ = 44.949 + 6.340\times10^{-3}T\ln T - 2.802\times10^{-6}T^2 + 27.675T^{-1} - 68.066\times10^{-3}T$

750-1728 K: $\Delta Hf^\circ = 42.039 - 0.092\times10^{-3}T - 1.100\times10^{-6}T^2 + 368.950T^{-1}$

$\Delta Gf^\circ = 42.039 + 0.092\times10^{-3}T\ln T + 1.100\times10^{-6}T^2 + 184.475T^{-1} - 26.023\times10^{-3}T$

1728-2000 K: $\Delta Hf^\circ = 41.974 - 4.321\times10^{-3}T + 0.057\times10^{-6}T^2 + 55.350T^{-1}$

$\Delta Gf^\circ = 41.974 + 4.321\times10^{-3}T\ln T - 0.057\times10^{-6}T^2 + 27.675T^{-1} - 55.459\times10^{-3}T$

Source: Data from Mah (150).

$NiCl_2$(c,l)
Nickel Dichloride
[Formation: Ni(c) + Cl_2(g) = $NiCl_2$(c,l)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	17.130	23.424	23.424	0	-72.980	-61.947	45.408
300	17.150	23.530	23.424	.032	-72.975	-61.878	45.078
400	18.167	28.616	24.111	1.802	-72.687	-58.223	31.811
500	18.753	32.739	25.437	3.651	-72.401	-54.641	23.883
600	19.085	36.190	26.950	5.544	-72.159	-51.115	18.618
631	19.146	37.153	27.428	6.137	-72.107	-50.027	17.327
700	19.281	39.148	28.487	7.463	-71.916	-47.620	14.868
800	19.446	41.733	29.983	9.400	-71.602	-44.174	12.068
900	19.677	44.036	31.419	11.355	-71.285	-40.765	9.899
1000	20.067	46.128	32.788	13.340	-70.956	-37.396	8.173
1100	20.709	48.068	34.089	15.377	-70.594	-34.046	6.764
1200	21.697	49.909	35.331	17.494	-70.173	-30.745	5.599
1300	23.122	51.699	36.522	19.730	-69.654	-27.483	4.620
1304	23.189	51.770	36.568	19.823	-69.630	-27.353	4.584
1304	23.900	65.932	36.568	38.290	-51.163	-27.353	4.584
1400	23.900	67.630	38.641	40.584	-50.539	-25.622	4.000

Phase changes: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
1230 ± 5 K, calculated sublimation point of $NiCl_2$; ΔH° = 52.7 kcal/mol.
1304 K, melting point of $NiCl_2$; ΔH° = 18.467 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1304 K: $Cp^\circ = 17.492 + 3.136\times10^{-3}T - 1.151\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 17.492\times10^{-3}T + 1.568\times10^{-6}T^2 + 1.151\times10^{2}T^{-1} - 5.741$
1304-1400 K: $Cp^\circ = 23.900$
$H^\circ - H^\circ_{298} = 23.900\times10^{-3}T + 7.124$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf^\circ = -74.776 + 5.669\times10^{-3}T - 2.800\times10^{-6}T^2 + 105.800T^{-1}$
$\Delta Gf^\circ = -74.776 - 5.669\times10^{-3}T\ln T + 2.800\times10^{-6}T^2 + 52.900T^{-1} + 73.900\times10^{-3}T$
631-750 K: $\Delta Hf^\circ = -72.227 - 2.655\times10^{-3}T + 4.225\times10^{-6}T^2 + 46.800T^{-1}$
$\Delta Gf^\circ = -72.227 + 2.655\times10^{-3}T\ln T - 4.225\times10^{-6}T^2 + 23.400T^{-1} + 20.700\times10^{-3}T$
750-1304 K: $\Delta Hf^\circ = -75.137 + 3.594\times10^{-3}T + 0.323\times10^{-6}T^2 + 360.400T^{-1}$
$\Delta Gf^\circ = -75.137 - 3.594\times10^{-3}T\ln T - 0.323\times10^{-6}T^2 + 180.200T^{-1} + 62.744\times10^{-3}T$
1304-1400 K: $\Delta Hf^\circ = -62.272 + 10.002\times10^{-3}T - 1.245\times10^{-6}T^2 + 245.300T^{-1}$
$\Delta Gf^\circ = -62.272 - 10.002\times10^{-3}T\ln T + 1.245\times10^{-6}T^2 + 122.650T^{-1} + 96.833\times10^{-3}T$

Source: Data from Mah (150).

$NiCl_2(g)$

Nickel Dichloride (ideal gas)

[Formation: $Ni(c,l) + Cl_2(g) = NiCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	14.487	71.252	71.252	0	-16.800	-20.027	14.680
300	14.504	71.341	71.251	.027	-16.800	-20.046	14.604
400	15.204	75.620	71.830	1.516	-16.793	-21.131	11.545
500	15.581	79.058	72.944	3.057	-16.815	-22.214	9.710
600	15.780	81.918	74.208	4.626	-16.897	-23.290	8.483
631	15.809	82.714	74.606	5.116	-16.948	-23.617	8.180
700	15.875	84.359	75.488	6.210	-16.989	-24.341	7.600
800	15.911	86.482	76.733	7.799	-17.023	-25.394	6.937
900	15.916	88.356	77.922	9.391	-17.069	-26.437	6.420
1000	15.909	90.033	79.051	10.982	-17.134	-27.479	6.005
1100	15.900	91.549	80.119	12.573	-17.218	-28.500	5.662
1200	15.894	92.932	81.130	14.162	-17.325	-29.524	5.377
1300	15.893	94.204	82.087	15.752	-17.452	-30.538	5.134
1400	15.896	95.382	82.996	17.341	-17.602	-31.538	4.923
1500	15.902	96.479	83.858	18.931	-17.775	-32.529	4.739
1600	15.911	97.505	84.679	20.522	-17.972	-33.502	4.576
1700	15.921	98.470	85.462	22.113	-18.192	-34.476	4.432
1728	15.924	98.730	85.675	22.559	-18.258	-34.729	4.392
1728	15.924	98.730	85.675	22.559	-22.358	-34.729	4.392
1800	15.932	99.381	86.211	23.706	-22.537	-35.245	4.279
1900	15.942	100.242	86.926	25.300	-22.785	-35.946	4.135
2000	15.952	101.060	87.613	26.894	-23.036	-36.628	4.002

Phase changes: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
1728 K, melting point of Ni; ΔH° = 4.100 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 16.321 - 0.232\times10^{-3}T - 1.569\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 16.321\times10^{-3}T - 0.116\times10^{-6}T^2 + 1.569\times10^{2}T^{-1} - 5.382$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf^\circ = -18.238 + 4.498\times10^{-3}T - 4.484\times10^{-6}T^2 + 147.600T^{-1}$

$\Delta Gf^\circ = -18.238 - 4.498\times10^{-3}T\ln T + 4.484\times10^{-6}T^2 + 73.800T^{-1} + 17.460\times10^{-3}T$

631-750 K: $\Delta Hf^\circ = -15.689 - 3.826\times10^{-3}T + 2.541\times10^{-6}T^2 + 88.600T^{-1}$

$\Delta Gf^\circ = -15.689 + 3.826\times10^{-3}T\ln T - 2.541\times10^{-6}T^2 + 44.300T^{-1} - 35.740\times10^{-3}T$

750-1728 K: $\Delta Hf^\circ = -18.599 + 2.423\times10^{-3}T - 1.361\times10^{-6}T^2 + 402.200T^{-1}$

$\Delta Gf^\circ = -18.599 - 2.423\times10^{-3}T\ln T + 1.361\times10^{-6}T^2 + 201.100T^{-1} + 6.304\times10^{-3}T$

1728-2000 K: $\Delta Hf^\circ = -18.664 - 1.806\times10^{-3}T - 0.204\times10^{-6}T^2 + 88.600T^{-1}$

$\Delta Gf^\circ = -18.664 + 1.806\times10^{-3}T\ln T + 0.204\times10^{-6}T^2 + 44.300T^{-1} - 23.132\times10^{-3}T$

Source: Data from Mah (150).

NiF(g)
Nickel Monofluoride (ideal gas)
[Formation: $Ni(c,l) + 0.5F_2(g) = NiF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	7.795	57.249	57.249	0	25.000	17.282	-12.668
300	7.806	57.298	57.251	.014	24.995	17.233	-12.554
400	8.310	59.614	57.561	.821	24.765	14.680	-8.021
500	8.712	61.514	58.168	1.673	24.506	12.187	-5.327
600	9.009	63.130	58.863	2.560	24.195	9.749	-3.551
631	9.073	63.585	59.084	2.840	24.076	9.007	-3.120
700	9.215	64.535	59.575	3.472	23.885	7.373	-2.302
800	9.350	65.775	60.275	4.400	23.646	5.026	-1.373
900	9.435	66.882	60.949	5.340	23.402	2.713	-.659
1000	9.486	67.879	61.593	6.286	23.146	.425	-.093
1100	9.515	68.784	62.206	7.236	22.875	-1.824	.362
1200	9.534	69.613	62.789	8.189	22.587	-4.060	.739
1300	9.550	70.377	63.344	9.143	22.278	-6.271	1.054
1400	9.569	71.085	63.871	10.099	21.949	-8.453	1.320
1500	9.593	71.746	64.375	11.057	21.598	-10.615	1.547
1600	9.627	72.366	64.855	12.018	21.227	-12.746	1.741
1700	9.672	72.951	65.314	12.983	20.836	-14.869	1.911
1728	9.688	73.109	65.439	13.254	20.722	-15.441	1.953
1728	9.688	73.109	65.439	13.254	16.622	-15.441	1.953
1800	9.728	73.506	65.754	13.953	16.322	-16.774	2.037
1900	9.795	74.033	66.176	14.929	15.912	-18.605	2.140
2000	9.873	74.538	66.582	15.912	15.506	-20.408	2.230

*Enthalpy of formation at 298 K estimated.

Phase changes: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
1728 K, melting point of Ni; ΔH° = 4.100 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 9.106 + 0.402\times10^{-3}T - 1.272\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 9.106\times10^{-3}T + 0.201\times10^{-6}T^2 + 1.272\times10^{2}T^{-1} - 3.159$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf^\circ = 24.361 + 1.856\times10^{-3}T - 4.166\times10^{-6}T^2 + 135.950T^{-1}$

$\Delta Gf^\circ = 24.361 - 1.856\times10^{-3}T\ln T + 4.166\times10^{-6}T^2 + 67.975T^{-1} - 15.176\times10^{-3}T$

631-750 K: $\Delta Hf^\circ = 26.910 - 6.468\times10^{-3}T + 2.859\times10^{-6}T^2 + 76.950T^{-1}$

$\Delta Gf^\circ = 26.910 + 6.468\times10^{-3}T\ln T - 2.859\times10^{-6}T^2 + 38.475T^{-1} - 68.376\times10^{-3}T$

750-1728 K: $\Delta Hf^\circ = 24.000 - 0.219\times10^{-3}T - 1.043\times10^{-6}T^2 + 390.550T^{-1}$

$\Delta Gf^\circ = 24.000 + 0.219\times10^{-3}T\ln T + 1.043\times10^{-6}T^2 + 195.275T^{-1} - 26.333\times10^{-3}T$

1728-2000 K: $\Delta Hf^\circ = 23.934 - 4.448\times10^{-3}T + 0.114\times10^{-6}T^2 + 76.950T^{-1}$

$\Delta Gf^\circ = 23.934 + 4.448\times10^{-3}T\ln T - 0.114\times10^{-6}T^2 + 38.475T^{-1} - 55.769\times10^{-3}T$

Source: Data from Mah (150) who estimated enthalpy of formation at 298 K and some molecular constants.

$NiF_2(c)$
Nickel Difluoride
[Formation: $Ni(c) + F_2(g) = NiF_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	15.310	17.590	17.590	0	-157.200	-145.872	106.926
300	15.345	17.685	17.592	.028	-157.198	-145.803	106.216
400	16.500	22.285	18.210	1.630	-157.017	-142.031	77.601
500	17.051	26.030	19.410	3.310	-156.851	-138.304	60.452
600	17.468	29.177	20.784	5.036	-156.737	-134.610	49.031
631	17.588	30.060	21.218	5.579	-156.724	-133.466	46.226
700	17.855	31.899	22.182	6.802	-156.617	-130.925	40.876
800	18.230	34.308	23.549	8.607	-156.411	-127.272	34.769
900	18.593	36.476	24.867	10.448	-156.189	-123.642	30.024
1000	18.948	38.453	26.128	12.325	-155.954	-120.042	26.235
1100	19.310	40.276	27.332	14.238	-155.705	-116.453	23.137
1200	19.707	41.973	28.483	16.188	-155.442	-112.900	20.562
1300	20.180	43.568	29.582	18.182	-155.158	-109.367	18.386
1400	20.797	45.085	30.636	20.229	-154.846	-105.856	16.525
1500	21.648	46.548	31.649	22.349	-154.486	-102.371	14.915
1600	22.864	47.981	32.624	24.571	-154.050	-98.906	13.510

Phase change: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1600 K: $Cp^\circ = 15.917 + 3.332\times10^{-3}T - 1.423\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 15.917\times10^{-3}T + 1.666\times10^{-6}T^2 + 1.423\times10^{2}T^{-1} - 5.371$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf^\circ = -158.606 + 4.413\times10^{-3}T - 2.788\times10^{-6}T^2 + 100.800T^{-1}$

$\Delta Gf^\circ = -158.606 - 4.413\times10^{-3}T\ln T + 2.788\times10^{-6}T^2 + 50.400T^{-1} + 66.454\times10^{-3}T$

631-750 K: $\Delta Hf^\circ = -156.057 - 3.911\times10^{-3}T + 4.237\times10^{-6}T^2 + 41.800T^{-1}$

$\Delta Gf^\circ = -156.057 + 3.911\times10^{-3}T\ln T - 4.237\times10^{-6}T^2 + 20.900T^{-1} + 13.254\times10^{-3}T$

750-1600 K: $\Delta Hf^\circ = -158.967 + 2.338\times10^{-3}T + 0.335\times10^{-6}T^2 + 355.400T^{-1}$

$\Delta Gf^\circ = -158.967 - 2.338\times10^{-3}T\ln T - 0.335\times10^{-6}T^2 + 177.700T^{-1} + 55.298\times10^{-3}T$

Source: Data from Mah (150).

$NiF_2(g)$

Nickel Difluoride (ideal gas)

[Formation: $Ni(c,l) + F_2(g) = NiF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.555	65.238	65.238	0	-80.200	-83.079	60.897
300	12.576	65.316	65.239	.023	-80.203	-83.097	60.535
400	13.549	69.074	65.744	1.332	-80.315	-84.045	45.919
500	14.264	72.178	66.730	2.724	-80.437	-84.964	37.137
600	14.773	74.827	67.864	4.178	-80.595	-85.858	31.273
631	14.882	75.574	68.224	4.638	-80.665	-86.127	29.830
700	15.124	77.132	69.026	5.674	-80.745	-86.716	27.074
800	15.356	79.168	70.169	7.199	-80.819	-87.568	23.922
900	15.499	80.985	71.272	8.742	-80.895	-88.406	21.468
1000	15.580	82.623	72.327	10.296	-80.983	-89.241	19.503
1100	15.617	84.110	73.331	11.857	-81.086	-90.051	17.891
1200	15.627	85.469	74.286	13.419	-81.211	-90.864	16.548
1300	15.617	86.720	75.196	14.981	-81.359	-91.665	15.410
1400	15.596	87.877	76.061	16.542	-81.533	-92.452	14.432
1500	15.568	88.952	76.885	18.100	-81.735	-93.227	13.583
1600	15.537	89.955	77.670	19.656	-81.965	-93.979	12.837
1700	15.504	90.896	78.421	21.208	-82.223	-94.733	12.179
1728	15.495	91.149	78.625	21.642	-82.301	-94.924	12.005
1728	15.495	91.149	78.625	21.642	-86.401	-94.924	12.005
1800	15.471	91.782	79.140	22.756	-86.614	-95.279	11.568
1900	15.439	92.617	79.826	24.302	-86.911	-95.755	11.014
2000	15.408	93.408	80.486	25.844	-87.216	-96.208	10.513

Phase changes: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
1728 K, melting point of Ni; ΔH° = 4.100 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 15.370 + 0.248\times10^{-3}T - 2.568\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 15.370\times10^{-3}T + 0.124\times10^{-6}T^2 + 2.568\times10^{2}T^{-1} - 5.455$

Formation equations (kcal/mol):

298.15-631 K: $\Delta Hf^\circ = -81.690 + 3.866\times10^{-3}T - 4.330\times10^{-6}T^2 + 215.300T^{-1}$

$\Delta Gf^\circ = -81.690 - 3.866\times10^{-3}T\ln T + 4.330\times10^{-6}T^2 + 107.650T^{-1} + 14.867\times10^{-3}T$

631-750 K: $\Delta Hf^\circ = -79.141 - 4.458\times10^{-3}T + 2.695\times10^{-6}T^2 + 156.300T^{-1}$

$\Delta Gf^\circ = -79.141 + 4.458\times10^{-3}T\ln T - 2.695\times10^{-6}T^2 + 78.150T^{-1} - 38.333\times10^{-3}T$

750-1728 K: $\Delta Hf^\circ = -82.051 + 1.791\times10^{-3}T - 1.207\times10^{-6}T^2 + 469.900T^{-1}$

$\Delta Gf^\circ = -82.051 - 1.791\times10^{-3}T\ln T + 1.207\times10^{-6}T^2 + 234.950T^{-1} + 3.711\times10^{-3}T$

1728-2000 K: $\Delta Hf^\circ = -82.117 - 2.438\times10^{-3}T - 0.050\times10^{-6}T^2 + 156.300T^{-1}$

$\Delta Gf^\circ = -82.117 + 2.438\times10^{-3}T\ln T + 0.050\times10^{-6}T^2 + 78.150T^{-1} - 25.726\times10^{-3}T$

Source: Data from Mah (150).

NiI(g)

Nickel Monoiodide (ideal gas)

[Formation: $Ni(c,l) + 0.5I_2(c,l,g) = NiI(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.754	64.558	64.558	0	59.000	46.019	-33.732
300	8.758	64.612	64.559	.016	58.992	45.938	-33.466
386.8	8.969	66.864	64.834	.785	58.595	42.210	-23.849
386.8	8.969	66.864	64.834	.785	56.740	42.210	-23.849
400	9.001	67.166	64.906	.904	56.642	41.716	-22.792
458.4	9.126	68.401	65.272	1.435	56.203	39.569	-18.865
458.4	9.126	68.401	65.272	1.435	51.193	39.569	-18.865
500	9.215	69.198	65.566	1.816	51.085	38.519	-16.837
600	9.385	70.894	66.317	2.746	50.785	36.030	-13.124
631	9.423	71.368	66.554	3.038	50.668	35.273	-12.217
700	9.506	72.350	67.077	3.691	50.482	33.603	-10.491
800	9.581	73.625	67.817	4.646	50.250	31.204	-8.525
900	9.623	74.756	68.527	5.606	50.010	28.837	-7.002
1000	9.642	75.771	69.202	6.569	49.758	26.494	-5.790
1100	9.647	76.690	69.841	7.534	49.491	24.191	-4.806
1200	9.648	77.530	70.448	8.499	49.206	21.900	-3.988
1300	9.649	78.302	71.023	9.463	48.900	19.634	-3.301
1400	9.656	79.017	71.568	10.429	48.576	17.398	-2.716
1500	9.671	79.684	72.087	11.395	48.228	15.179	-2.212
1600	9.698	80.309	72.582	12.363	47.859	12.992	-1.775
1700	9.736	80.898	73.054	13.335	47.471	10.813	-1.390
1728	9.750	81.057	73.182	13.608	47.358	10.226	-1.293
1728	9.750	81.057	73.182	13.608	43.258	10.226	-1.293
1800	9.787	81.456	73.505	14.311	42.961	8.852	-1.075
1900	9.850	81.987	73.938	15.293	42.554	6.963	-.801
2000	9.924	82.494	74.354	16.281	42.152	5.106	-.558

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
1728 K, melting point of Ni; ΔH° = 4.100 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 9.440 + 0.204\times10^{-3}T - 0.664\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 9.440\times10^{-3}T + 0.102\times10^{-6}T^2 + 0.664\times10^{2}T^{-1} - 3.046$

NiI(g) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = 59.015 + 0.005\times10^{-3}T - 4.924\times10^{-6}T^2 + 125.400T^{-1}$

$\Delta Gf^\circ = 59.015 - 0.005\times10^{-3}T\ln T + 4.924\times10^{-6}T^2 + 62.700T^{-1} - 45.733\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = 58.288 - 3.197\times10^{-3}T - 4.178\times10^{-6}T^2 + 125.400T^{-1}$

$\Delta Gf^\circ = 58.288 + 3.197\times10^{-3}T\ln T + 4.178\times10^{-6}T^2 + 62.700T^{-1} - 62.641\times10^{-3}T$

458.4-631 K: $\Delta Hf^\circ = 50.931 + 1.973\times10^{-3}T - 4.212\times10^{-6}T^2 + 117.750T^{-1}$

$\Delta Gf^\circ = 50.931 - 1.973\times10^{-3}T\ln T + 4.212\times10^{-6}T^2 + 58.875T^{-1} - 14.909\times10^{-3}T$

631-750 K: $\Delta Hf^\circ = 53.480 - 6.351\times10^{-3}T + 2.813\times10^{-6}T^2 + 58.750T^{-1}$

$\Delta Gf^\circ = 53.480 + 6.351\times10^{-3}T\ln T - 2.813\times10^{-6}T^2 + 29.375T^{-1} - 68.109\times10^{-3}T$

750-1728 K: $\Delta Hf^\circ = 50.570 - 0.102\times10^{-3}T - 1.089\times10^{-6}T^2 + 372.350T^{-1}$

$\Delta Gf^\circ = 50.570 + 0.102\times10^{-3}T\ln T + 1.089\times10^{-6}T^2 + 186.175T^{-1} - 26.066\times10^{-3}T$

1728-2000 K: $\Delta Hf^\circ = 50.505 - 4.331\times10^{-3}T + 0.068\times10^{-6}T^2 + 58.750T^{-1}$

$\Delta Gf^\circ = 50.505 + 4.331\times10^{-3}T\ln T - 0.068\times10^{-6}T^2 + 29.375T^{-1} - 55.502\times10^{-3}T$

Source: Data from Mah (150) who estimated some molecular constants.

NiI_2(c)
Nickel Diiodide
[Formation: $Ni(c) + I_2(c,l,g) = NiI_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.500	33.150	33.150	0	-18.700	-18.179	13.325
300	18.513	33.265	33.152	.034	-18.702	-18.176	13.241
386.8	19.003	38.033	33.732	1.664	-18.843	-18.010	10.176
386.8	19.003	38.033	33.732	1.664	-22.552	-18.010	10.176
400	19.077	38.672	33.885	1.915	-22.645	-17.853	9.754
458.4	19.288	41.290	34.664	3.038	-23.054	-17.123	8.164
458.4	19.288	41.290	34.664	3.038	-33.075	-17.123	8.164
500	19.438	42.972	35.286	3.843	-32.945	-15.680	6.853
600*	19.618	46.534	36.872	5.797	-32.670	-12.256	4.464

*Vaporizes with decomposition above 600 K.

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp° = 19.108 + 1.326\times10^{-3}T - 0.892\times10^{5}T^{-2}$

$H°- H°_{298} = 19.108\times10^{-3}T + 0.663\times10^{-6}T^2 + 0.892\times10^{2}T^{-1} - 6.055$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -19.707 + 3.235\times10^{-3}T - 5.109\times10^{-6}T^2 + 148.200T^{-1}$

$\Delta Gf° = -19.707 - 3.235\times10^{-3}T\ln T + 5.109\times10^{-6}T^2 + 74.100T^{-1} + 21.202\times10^{-3}T$

386.8-458.4 K: $\Delta Hf° = -21.163 - 3.169\times10^{-3}T - 3.617\times10^{-6}T^2 + 148.200T^{-1}$

$\Delta Gf° = -21.163 + 3.169\times10^{-3}T\ln T + 3.617\times10^{-6}T^2 + 74.100T^{-1} - 12.613\times10^{-3}T$

458.4-600 K: $\Delta Hf° = -35.876 + 7.171\times10^{-3}T - 3.685\times10^{-6}T^2 + 132.900T^{-1}$

$\Delta Gf° = -35.876 - 7.171\times10^{-3}T\ln T + 3.685\times10^{-6}T^2 + 66.450T^{-1} + 82.849\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (253). Other data based on Worswick (268).

$NpF_6(c,l)$
Neptunium Hexafluoride
[Formation: $Np(c) + 3F_2(g) = NpF_6(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	40.020	54.755	54.755	0	-474.500	-443.900	325.383
300	40.170	55.003	54.756	.074	-474.481	-443.711	323.239
327.91	42.540	58.680	54.935	1.228	-474.161	-440.862	293.828
327.91	44.560	71.453	54.935	5.416	-469.973	-440.862	293.828
350	45.140	74.377	56.071	6.407	-469.648	-438.911	274.065

*Enthalpy of formation at 298 K estimated.

Phase changes: 327.91 K, melting point of NpF_6; ΔH° = 4.188 kcal/mol.
328.3 K, boiling point of NpF_6; ΔH° = 7 kcal/mol.
350 K, vapor pressure = 2 atm.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-327.91 K: $Cp^\circ = 15.105 + 83.564\times10^{-3}T$

$H^\circ - H^\circ_{298} = 15.105\times10^{-3}T + 41.782\times10^{-6}T^2 - 8.218$

327.91-350 K: $Cp^\circ = 36.049 + 26.000\times10^{-3}T$

$H^\circ - H^\circ_{298} = 36.049\times10^{-3}T + 13.000\times10^{-6}T^2 - 7.803$

Formation equations (kcal/mol):

298.15-327.91 K: $\Delta Hf^\circ = -474.083 - 9.516\times10^{-3}T + 31.449\times10^{-6}T^2 - 111.900T^{-1}$

$\Delta Gf^\circ = -474.083 + 9.516\times10^{-3}T\ln T - 31.449\times10^{-6}T^2 - 55.950T^{-1} + 57.023\times10^{-3}T$

327.91-350 K: $\Delta Hf^\circ = -473.668 + 11.428\times10^{-3}T + 2.667\times10^{-6}T^2 - 111.900T^{-1}$

$\Delta Gf^\circ = -473.668 - 11.428\times10^{-3}T\ln T - 2.667\times10^{-6}T^2 - 55.950T^{-1} + 167.643\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Weinstock (259) and estimates of Fuger (83). Other data from Osborne (181).

$NpF_6(g)$

Neptunium Hexafluoride (ideal gas)

[Formation: $Np(c,l) + 3F_2(g) = NpF_6(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	30.848	89.991	89.991	0	-463.000	-442.905	324.654
300	30.909	90.182	89.992	.057	-462.998	-442.781	322.562
400	33.366	99.446	91.239	3.283	-462.833	-436.065	238.252
500	34.755	107.054	93.662	6.696	-462.720	-429.387	187.683
553	35.199	110.584	95.118	8.552	-462.712	-425.857	168.300
553	35.199	110.584	95.118	8.552	-464.052	-425.857	168.300
600	35.592	113.471	96.444	10.216	-464.007	-422.612	153.934
700	36.129	119.001	99.281	13.804	-463.903	-415.721	129.792
800	36.492	123.850	102.055	17.436	-463.797	-408.847	111.690
849	36.618	126.023	103.376	19.227	-463.745	-405.483	104.378
849	36.618	126.023	103.376	19.227	-465.005	-405.483	104.378
900	36.750	128.164	104.721	21.099	-464.912	-401.907	97.595
912	36.773	128.651	105.032	21.540	-464.890	-401.066	96.109
912	36.773	128.651	105.032	21.540	-466.130	-401.066	96.109
1000	36.943	132.046	107.262	24.784	-466.166	-394.790	86.280

*Enthalpy of formation at 298 K estimated.

Phase changes: 553 K, α - β transition point of Np; $\Delta H°$ = 1.340 kcal/mol.
849 K, β - γ transition point of Np; $\Delta H°$ = 1.260 kcal/mol.
912 K, melting point of Np; $\Delta H°$ = 1.240 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 35.833 + 1.724\times10^{-3}T - 4.888\times10^{5}T^{-2}$

$H°- H°_{298} = 35.833\times10^{-3}T + 0.862\times10^{-6}T^2 + 4.888\times10^{2}T^{-1} - 12.400$

Formation equations (kcal/mol):

298.15-553 K: $\Delta Hf° = -466.765 + 11.212\times10^{-3}T - 9.471\times10^{-6}T^2 + 376.900T^{-1}$

$\Delta Gf° = -466.765 - 11.212\times10^{-3}T\ln T + 9.471\times10^{-6}T^2 + 188.450T^{-1} + 138.964\times10^{-3}T$

553-849 K: $\Delta Hf° = -465.066 + 0.910\times10^{-3}T + 0.340\times10^{-6}T^2 + 187.300T^{-1}$

$\Delta Gf° = -465.066 - 0.910\times10^{-3}T\ln T - 0.340\times10^{-6}T^2 + 93.650T^{-1} + 76.565\times10^{-3}T$

849-912 K: $\Delta Hf° = -466.921 + 1.611\times10^{-3}T + 0.340\times10^{-6}T^2 + 187.300T^{-1}$

$\Delta Gf° = -466.921 - 1.611\times10^{-3}T\ln T - 0.340\times10^{-6}T^2 + 93.650T^{-1} + 83.478\times10^{-3}T$

912-1000 K: $\Delta Hf° = -466.198 - 0.541\times10^{-3}T + 0.340\times10^{-6}T^2 + 187.300T^{-1}$

$\Delta Gf° = -466.198 + 0.541\times10^{-3}T\ln T - 0.340\times10^{-6}T^2 + 93.650T^{-1} + 68.018\times10^{-3}T$

Sources: Enthalpy of formation at 298 K estimated by Fuger (83). Other data from Osborne (181).

PBr(g)

Phosphorus Monobromide (ideal gas)

[Formation: $P(c,l,1/4P_4(g)) + 0.5Br_2(l,g) = PBr(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	8.460	59.537	59.537	0	38.800	29.400	-21.551
300	8.465	59.589	59.537	.016	38.788	29.342	-21.375
317.3	8.502	60.065	59.552	.163	38.680	28.801	-19.837
317.3	8.502	60.065	59.552	.163	38.523	28.801	-19.837
332.6	8.534	60.466	59.585	.293	38.419	28.335	-18.618
332.6	8.534	60.466	59.585	.293	34.887	28.335	-18.618
400	8.677	62.057	59.872	.874	34.750	27.019	-14.762
500	8.792	64.007	60.511	1.748	34.554	25.108	-10.975
550	8.828	64.846	60.867	2.189	34.458	24.155	-9.598
550	8.828	64.846	60.867	2.189	31.550	24.155	-9.598
600	8.863	65.616	61.231	2.631	31.536	23.484	-8.554
700	8.912	66.986	61.957	3.520	31.507	22.145	-6.914
800	8.947	68.179	62.663	4.413	31.475	20.809	-5.685
900	8.975	69.234	63.335	5.309	31.439	19.478	-4.730
1000	8.999	70.181	63.973	6.208	31.403	18.151	-3.967
1100	9.019	71.040	64.577	7.109	31.366	16.827	-3.343
1200	9.037	71.825	65.148	8.012	31.329	15.508	-2.824
1300	9.054	72.549	65.691	8.916	31.290	14.190	-2.385
1400	9.069	73.221	66.205	9.822	31.252	12.876	-2.010
1500	9.083	73.847	66.694	10.730	31.214	11.564	-1.685
1600	9.097	74.434	67.160	11.639	31.176	10.256	-1.401
1700	9.111	74.986	67.604	12.549	31.138	8.948	-1.150
1800	9.124	75.507	68.029	13.461	31.102	7.645	-.928
1900	9.137	76.001	68.436	14.374	31.065	6.343	-.730
2000	9.149	76.469	68.825	15.288	31.029	5.044	-.551

*Data estimated.

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
550 K, boiling point of P to $P_4(g)$; ΔH° = 2.908 kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.897 + 0.138\times10^{-3}T - 0.425\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.897\times10^{-3}T + 0.069\times10^{-6}T^2 + 0.425\times10^{2}T^{-1} - 2.801$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf^\circ = 40.107 - 3.947\times10^{-3}T - 3.066\times10^{-6}T^2 + 42.500T^{-1}$

$\Delta Gf^\circ = 40.107 + 3.947\times10^{-3}T\ln T + 3.066\times10^{-6}T^2 + 21.250T^{-1} - 59.555\times10^{-3}T$

317.3-332.6 K: $\Delta Hf^\circ = 40.420 - 6.440\times10^{-3}T + 0.119\times10^{-6}T^2 + 42.500T^{-1}$

$\Delta Gf^\circ = 40.420 + 6.440\times10^{-3}T\ln T - 0.119\times10^{-6}T^2 + 21.250T^{-1} - 73.892\times10^{-3}T$

332.6-550 K: $\Delta Hf^\circ = 35.420 - 1.860\times10^{-3}T + 0.042\times10^{-6}T^2 + 26.800T^{-1}$

$\Delta Gf^\circ = 35.420 + 1.860\times10^{-3}T\ln T - 0.042\times10^{-6}T^2 + 13.400T^{-1} - 32.214\times10^{-3}T$

550-2000 K: $\Delta Hf^\circ = 31.960 - 0.522\times10^{-3}T + 0.038\times10^{-6}T^2 - 73.500T^{-1}$

$\Delta Gf^\circ = 31.960 + 0.522\times10^{-3}T\ln T - 0.038\times10^{-6}T^2 - 36.750T^{-1} - 17.317\times10^{-3}T$

Source: Data from JANAF (60) except enthalpy of formation at 298 K converted to P(white) standard state.

$PBr_3(g)$

Phosphorus Tribromide (ideal gas)

[Formation: $P(c,l,1/4P_4(g)) + 1.5Br_2(l,g) = PBr_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	18.173	83.206	83.206	0	-34.900	-40.510	29.695
300	18.191	83.318	83.206	.034	-34.927	-40.544	29.536
317.3	18.307	84.341	83.239	.350	-35.178	-40.861	28.144
317.3	18.307	84.341	83.239	.350	-35.335	-40.861	28.144
332.6	18.410	85.206	83.310	.631	-35.564	-41.122	27.021
332.6	18.410	85.206	83.310	.631	-46.162	-41.122	27.021
400	18.863	88.655	83.930	1.890	-46.210	-40.101	21.910
500	19.206	92.905	85.313	3.796	-46.256	-38.567	16.858
550	19.304	94.742	86.089	4.759	-46.272	-37.812	15.025
550	19.304	94.742	86.089	4.759	-49.180	-37.812	15.025
600	19.402	96.426	86.881	5.727	-49.113	-36.781	13.397
700	19.523	99.427	88.464	7.674	-48.977	-34.736	10.845
800	19.603	102.039	90.002	9.630	-48.842	-32.710	8.936
900	19.659	104.352	91.471	11.593	-48.709	-30.704	7.456
1000	19.699	106.425	92.864	13.561	-48.576	-28.710	6.274
1100	19.729	108.304	94.183	15.533	-48.444	-26.729	5.310
1200	19.751	110.022	95.433	17.507	-48.314	-24.761	4.510
1300	19.769	111.603	96.616	19.483	-48.185	-22.804	3.834
1400	19.783	113.069	97.740	21.461	-48.057	-20.855	3.256
1500	19.795	114.434	98.807	23.440	-47.932	-18.918	2.756
1600	19.804	115.712	99.825	25.420	-47.808	-16.986	2.320
1700	19.812	116.913	100.795	27.400	-47.686	-15.066	1.937
1800	19.818	118.045	101.722	29.382	-47.563	-13.148	1.596
1900	19.824	119.117	102.610	31.364	-47.443	-11.238	1.293
2000	19.829	120.134	103.461	33.347	-47.324	-9.337	1.020

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
550 K, boiling point of P to $P_4(g)$; ΔH° = 2.908 kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.739 + 0.084\times10^{-3}T - 1.414\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.739\times10^{-3}T + 0.042\times10^{-6}T^2 + 1.414\times10^{2}T^{-1} - 6.363$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf^\circ = -31.770 - 11.196\times10^{-3}T - 2.993\times10^{-6}T^2 + 141.400T^{-1}$

$\Delta Gf^\circ = -31.770 + 11.196\times10^{-3}T\ln T + 2.993\times10^{-6}T^2 + 70.700T^{-1} - 94.797\times10^{-3}T$

317.3-332.6 K: $\Delta Hf^\circ = -31.457 - 13.689\times10^{-3}T + 0.192\times10^{-6}T^2 + 141.400T^{-1}$

$\Delta Gf^\circ = -31.457 + 13.689\times10^{-3}T\ln T - 0.192\times10^{-6}T^2 + 70.700T^{-1} - 109.133\times10^{-3}T$

332.6-550 K: $\Delta Hf^\circ = -46.457 + 0.052\times10^{-3}T - 0.041\times10^{-6}T^2 + 94.300T^{-1}$

$\Delta Gf^\circ = -46.457 - 0.052\times10^{-3}T\ln T + 0.041\times10^{-6}T^2 + 47.150T^{-1} + 15.900\times10^{-3}T$

550-2000 K: $\Delta Hf^\circ = -49.918 + 1.390\times10^{-3}T - 0.045\times10^{-6}T^2 - 6.000T^{-1}$

$\Delta Gf^\circ = -49.918 - 1.390\times10^{-3}T\ln T + 0.045\times10^{-6}T^2 - 3.000T^{-1} + 30.798\times10^{-3}T$

Source: Data from JANAF (60) except enthalpy of formation at 298 K converted to P(white) standard state.

PCl(g)

Phosphorus Monochloride (ideal gas)

[Formation: $P(c,1,1/4P_4(g)) + 0.5Cl_2(g) = PCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	8.298	56.829	56.829	0	30.800	24.728	-18.126
300	8.305	56.881	56.831	.015	30.796	24.690	-17.986
317.3	8.350	57.348	56.847	.159	30.771	24.339	-16.764
317.3	8.350	57.348	56.847	.159	30.614	24.339	-16.764
400	8.566	59.310	57.160	.860	30.451	22.724	-12.416
500	8.712	61.238	57.788	1.725	30.260	20.816	-9.098
550	8.757	62.071	58.140	2.162	30.165	19.861	-7.892
550	8.757	62.071	58.140	2.162	27.257	19.861	-7.892
600	8.801	62.835	58.500	2.601	27.246	19.190	-6.990
700	8.861	64.197	59.220	3.484	27.218	17.849	-5.573
800	8.904	65.383	59.918	4.372	27.185	16.513	-4.511
900	8.937	66.433	60.583	5.265	27.150	15.183	-3.687
1000	8.964	67.376	61.216	6.160	27.113	13.854	-3.028
1100	8.986	68.232	61.817	7.057	27.075	12.529	-2.489
1200	9.005	69.015	62.384	7.957	27.036	11.208	-2.041
1300	9.022	69.736	62.922	8.858	26.996	9.891	-1.663
1400	9.038	70.405	63.433	9.761	26.956	8.577	-1.339
1500	9.052	71.029	63.918	10.666	26.916	7.265	-1.059
1600	9.066	71.614	64.382	11.571	26.875	5.956	-.814
1700	9.079	72.164	64.823	12.479	26.835	4.651	-.598
1800	9.091	72.683	65.246	13.387	26.795	3.347	-.406
1900	9.103	73.175	65.650	14.297	26.755	2.046	-.235
2000	9.114	73.642	66.038	15.208	26.715	.748	-.082

*Data estimated.

Phase changes: 317.3 K, melting point of P; $\Delta H° = 0.157$ kcal/mol.
550 K, boiling point of P to $P_4(g)$; $\Delta H° = 2.908$ kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.863 + 0.144\times10^{-3}T - 0.540\times10^{5}T^{-2}$

$H°-H°_{298} = 8.863\times10^{-3}T + 0.072\times10^{-6}T^2 + 0.540\times10^{2}T^{-1} - 2.830$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = 30.820 + 0.650\times10^{-3}T - 3.157\times10^{-6}T^2 + 19.850T^{-1}$

$\Delta Gf° = 30.820 - 0.650\times10^{-3}T\ln T + 3.157\times10^{-6}T^2 + 9.925T^{-1} - 17.778\times10^{-3}T$

317.3-550 K: $\Delta Hf° = 31.133 - 1.842\times10^{-3}T + 0.028\times10^{-6}T^2 + 19.850T^{-1}$

$\Delta Gf° = 31.133 + 1.842\times10^{-3}T\ln T - 0.028\times10^{-6}T^2 + 9.925T^{-1} - 32.114\times10^{-3}T$

550-2000 K: $\Delta Hf° = 27.673 - 0.505\times10^{-3}T + 0.024\times10^{-6}T^2 - 80.450T^{-1}$

$\Delta Gf° = 27.673 + 0.505\times10^{-3}T\ln T - 0.024\times10^{-6}T^2 - 40.225T^{-1} - 17.217\times10^{-3}T$

Source: Data are estimations from JANAF (60) except enthalpy of formation at 298 K converted to P(white) standard state.

$PCl_3(g)$

Phosphorus Trichloride (ideal gas)

[Formation: $P(c,l,1/4P_4(g)) + 1.5Cl_2(g) = PCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	17.108	74.467	74.467	0	-69.000	-64.442	47.237
300	17.135	74.573	74.467	.032	-69.002	-64.414	46.925
317.3	17.315	75.539	74.499	.330	-69.014	-64.148	44.183
317.3	17.315	75.539	74.499	.330	-69.171	-64.148	44.183
400	18.173	79.661	75.154	1.803	-69.251	-62.828	34.327
500	18.731	83.782	76.480	3.651	-69.312	-61.214	26.756
550	18.894	85.577	77.227	4.592	-69.336	-60.418	24.008
550	18.894	85.577	77.227	4.592	-72.244	-60.418	24.008
600	19.057	87.228	77.993	5.541	-72.182	-59.345	21.616
700	19.263	90.182	79.528	7.458	-72.053	-57.215	17.863
800	19.401	92.764	81.024	9.392	-71.927	-55.105	15.054
900	19.497	95.055	82.458	11.337	-71.799	-53.009	12.872
1000	19.566	97.113	83.823	13.290	-71.672	-50.929	11.130
1100	19.618	98.980	85.116	15.250	-71.544	-48.860	9.708
1200	19.658	100.689	86.344	17.214	-71.419	-46.805	8.524
1300	19.689	102.264	87.509	19.181	-71.295	-44.759	7.525
1400	19.714	103.724	88.616	21.151	-71.172	-42.723	6.669
1500	19.734	105.085	89.669	23.124	-71.050	-40.695	5.929
1600	19.751	106.359	90.673	25.098	-70.930	-38.675	5.283
1700	19.764	107.557	91.631	27.074	-70.811	-36.660	4.713
1800	19.776	108.687	92.548	29.051	-70.693	-34.656	4.208
1900	19.786	109.756	93.425	31.029	-70.577	-32.654	3.756
2000	19.794	110.771	94.267	33.008	-70.464	-30.662	3.350

Phase changes: 317.3 K, melting point of P; $\Delta H°$ = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; $\Delta H°$ = 2.908 kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.571 + 0.178\times10^{-3}T - 2.236\times10^{5}T^{-2}$

$H°- H°_{298} = 19.571\times10^{-3}T + 0.089\times10^{-6}T^2 + 2.236\times10^{2}T^{-1} - 6.593$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = -69.874 + 2.531\times10^{-3}T - 3.228\times10^{-6}T^2 + 121.150T^{-1}$

$\Delta Gf° = -69.874 - 2.531\times10^{-3}T\ln T + 3.228\times10^{-6}T^2 + 60.575T^{-1} + 31.000\times10^{-3}T$

317.3-550 K: $\Delta Hf° = -69.561 + 0.038\times10^{-3}T - 0.043\times10^{-6}T^2 + 121.150T^{-1}$

$\Delta Gf° = -69.561 - 0.038\times10^{-3}T\ln T + 0.043\times10^{-6}T^2 + 60.575T^{-1} + 16.663\times10^{-3}T$

550-2000 K: $\Delta Hf° = -73.021 + 1.376\times10^{-3}T - 0.047\times10^{-6}T^2 + 20.850T^{-1}$

$\Delta Gf° = -73.021 - 1.376\times10^{-3}T\ln T + 0.047\times10^{-6}T^2 + 10.425T^{-1} + 31.561\times10^{-3}T$

Source: Data from JANAF (60) except enthalpy of formation at 298 K converted to P(white) standard state.

$PCl_5(g)$

Phosphorus Pentachloride (ideal gas)

[Formation: $P(c,1,1/4P_4(g)) + 2.5Cl_2(g) = PCl_5(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	26.743	87.043	87.043	0	-89.600	-72.903	53.439
300	26.792	87.209	87.043	.050	-89.598	-72.800	53.034
317.3	27.122	88.720	87.093	.516	-89.583	-71.830	49.475
317.3	27.122	88.720	87.093	.516	-89.740	-71.830	49.475
400	28.698	95.208	88.120	2.835	-89.664	-67.170	36.700
500	29.717	101.732	90.212	5.760	-89.501	-61.563	26.909
550	30.015	104.582	91.390	7.256	-89.404	-58.789	23.360
550	30.015	104.582	91.390	7.256	-92.312	-58.789	23.360
600	30.313	107.207	92.600	8.764	-92.125	-55.748	20.306
700	30.688	111.910	95.030	11.816	-91.740	-49.715	15.522
800	30.939	116.025	97.403	14.898	-91.351	-43.740	11.949
900	31.114	119.680	99.679	18.001	-90.955	-37.811	9.182
1000	31.240	122.965	101.846	21.119	-90.558	-31.929	6.978
1100	31.335	125.947	103.903	24.248	-90.158	-26.086	5.183
1200	31.407	128.677	105.856	27.385	-89.760	-20.280	3.693
1300	31.464	131.193	107.709	30.529	-89.361	-14.506	2.439
1400	31.509	133.527	109.471	33.678	-88.963	-8.763	1.368
1500	31.546	135.702	111.149	36.830	-88.568	-3.049	.444
1600	31.576	137.739	112.747	39.987	-88.173	2.641	-.361
1700	31.601	139.654	114.275	43.145	-87.781	8.308	-1.068
1800	31.622	141.461	115.735	46.307	-87.389	13.947	-1.693
1900	31.640	143.171	117.134	49.470	-87.000	19.570	-2.251
2000	31.655	144.794	118.477	52.634	-86.617	25.167	-2.750

Phase changes: 317.3 K, melting point of P; $\Delta H°$ = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; $\Delta H°$ = 2.908 kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 31.262 + 0.314\times10^{-3}T - 4.100\times10^{5}T^{-2}$

$H°- H°_{298} = 31.262\times10^{-3}T + 0.157\times10^{-6}T^2 + 4.100\times10^{2}T^{-1} - 10.710$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = -91.722 + 5.396\times10^{-3}T - 3.248\times10^{-6}T^2 + 239.250T^{-1}$

$\Delta Gf° = -91.722 - 5.396\times10^{-3}T\ln T + 3.248\times10^{-6}T^2 + 119.625T^{-1} + 91.548\times10^{-3}T$

317.3-550 K: $\Delta Hf° = -91.409 + 2.903\times10^{-3}T - 0.063\times10^{-6}T^2 + 239.250T^{-1}$

$\Delta Gf° = -91.409 - 2.903\times10^{-3}T\ln T + 0.063\times10^{-6}T^2 + 119.625T^{-1} + 77.212\times10^{-3}T$

550-2000 K: $\Delta Hf° = -94.869 + 4.240\times10^{-3}T - 0.067\times10^{-6}T^2 + 138.950T^{-1}$

$\Delta Gf° = -94.869 - 4.240\times10^{-3}T\ln T + 0.067\times10^{-6}T^2 + 69.475T^{-1} + 92.109\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Other data from JANAF (60).

PF(g)

Phosphorus Monofluoride (ideal gas)

[Formation: $P(c,l,1/4P_4(g)) + 0.5F_2(g) = PF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	7.557	53.743	53.743	0	-12.518	-18.392	13.482
300	7.565	53.789	53.743	.014	-12.522	-18.429	13.425
317.3	7.633	54.215	53.757	.145	-12.555	-18.768	12.927
317.3	7.633	54.215	53.757	.145	-12.712	-18.768	12.927
400	7.956	56.022	54.044	.791	-12.905	-20.322	11.103
500	8.236	57.829	54.627	1.601	-13.127	-22.150	9.682
550	8.333	58.620	54.954	2.016	-13.233	-23.062	9.164
550	8.333	58.620	54.954	2.016	-16.141	-23.062	9.164
600	8.430	59.349	55.291	2.435	-16.163	-23.690	8.629
700	8.565	60.659	55.966	3.285	-16.209	-24.940	7.786
800	8.664	61.810	56.626	4.147	-16.257	-26.185	7.153
900	8.739	62.835	57.261	5.017	-16.304	-27.422	6.659
1000	8.799	63.759	57.865	5.894	-16.352	-28.655	6.263
1100	8.849	64.600	58.439	6.777	-16.399	-29.883	5.937
1200	8.895	65.372	58.985	7.664	-16.446	-31.108	5.665
1300	8.938	66.085	59.503	8.556	-16.492	-32.326	5.434
1400	8.980	66.749	59.998	9.452	-16.537	-33.543	5.236
1500	9.023	67.370	60.469	10.352	-16.580	-34.757	5.064
1600	9.066	67.954	60.919	11.256	-16.622	-35.967	4.913
1700	9.111	68.505	61.349	12.165	-16.660	-37.174	4.779
1800	9.156	69.027	61.761	13.078	-16.696	-38.380	4.660
1900	9.202	69.523	62.157	13.996	-16.728	-39.583	4.553
2000	9.249	69.996	62.537	14.919	-16.757	-40.785	4.457

*Enthalpy of formation at 298 K estimated.

Phase changes: 317.3 K, melting point of P; $\Delta H° = 0.157$ kcal/mol.
550 K, boiling point of P to $P_4(g)$; $\Delta H° = 2.908$ kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.329 + 0.506\times10^{-3}T - 0.821\times10^{5}T^{-2}$

$H°-H°_{298} = 8.329\times10^{-3}T + 0.253\times10^{-6}T^2 + 0.821\times10^{2}T^{-1} - 2.781$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = -12.439 + 0.276\times10^{-3}T - 3.019\times10^{-6}T^2 + 31.850T^{-1}$

$\Delta Gf° = -12.439 - 0.276\times10^{-3}T\ln T + 3.019\times10^{-6}T^2 + 15.925T^{-1} - 19.474\times10^{-3}T$

317.3-550 K: $\Delta Hf° = -12.125 - 2.217\times10^{-3}T + 0.166\times10^{-6}T^2 + 31.850T^{-1}$

$\Delta Gf° = -12.125 + 2.217\times10^{-3}T\ln T - 0.166\times10^{-6}T^2 + 15.925T^{-1} - 33.810\times10^{-3}T$

550-2000 K: $\Delta Hf° = -15.586 - 0.879\times10^{-3}T + 0.162\times10^{-6}T^2 - 68.450T^{-1}$

$\Delta Gf° = -15.586 + 0.879\times10^{-3}T\ln T - 0.162\times10^{-6}T^2 - 34.225T^{-1} - 18.913\times10^{-3}T$

Source: Data from Chase (24) whose estimated enthalpy of formation at 298 K was converted to P(white) standard state.

$PF_2(g)$

Phosphorus Difluoride (ideal gas)

[Formation: $P(c,l,1/4P_4(g)) + F_2(g) = PF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	10.688	62.822	62.822	0	-116.696	-118.055	86.536
300	10.708	62.888	62.822	.020	-116.701	-118.064	86.009
317.3	10.869	63.493	62.842	.207	-116.744	-118.141	81.372
317.3	10.869	63.493	62.842	.207	-116.901	-118.141	81.372
400	11.639	66.104	63.254	1.140	-117.126	-118.435	64.709
500	12.266	68.773	64.099	2.337	-117.362	-118.735	51.898
550	12.474	69.955	64.578	2.957	-117.470	-118.881	47.238
550	12.474	69.955	64.578	2.957	-120.378	-118.881	47.238
600	12.683	71.049	65.072	3.586	-120.399	-118.744	43.252
700	12.967	73.027	66.071	4.869	-120.436	-118.465	36.986
800	13.166	74.772	67.051	6.177	-120.468	-118.181	32.285
900	13.310	76.331	67.997	7.501	-120.497	-117.892	28.628
1000	13.416	77.739	68.902	8.837	-120.526	-117.602	25.702
1100	13.497	79.022	69.765	10.183	-120.553	-117.308	23.307
1200	13.560	80.199	70.586	11.536	-120.580	-117.012	21.311
1300	13.610	81.287	71.368	12.895	-120.606	-116.714	19.621
1400	13.650	82.297	72.113	14.258	-120.634	-116.414	18.173
1500	13.683	83.240	72.823	15.625	-120.662	-116.112	16.917
1600	13.709	84.124	73.503	16.994	-120.691	-115.808	15.818
1700	13.732	84.955	74.151	18.366	-120.720	-115.499	14.848
1800	13.751	85.741	74.774	19.740	-120.751	-115.193	13.986
1900	13.767	86.485	75.371	21.116	-120.782	-114.882	13.214
2000	13.781	87.191	75.944	22.494	-120.814	-114.570	12.519

*Data estimated.

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; ΔH° = 2.908 kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 12.888 + 0.608\times10^{-3}T - 2.117\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 12.888\times10^{-3}T + 0.304\times10^{-6}T^2 + 2.117\times10^{2}T^{-1} - 4.580$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf^\circ = -116.971 + 0.581\times10^{-3}T - 3.055\times10^{-6}T^2 + 111.200T^{-1}$

$\Delta Gf^\circ = -116.971 - 0.581\times10^{-3}T\ln T + 3.055\times10^{-6}T^2 + 55.600T^{-1} - 1.864\times10^{-3}T$

317.3-550 K: $\Delta Hf^\circ = -116.657 - 1.912\times10^{-3}T + 0.130\times10^{-6}T^2 + 111.200T^{-1}$

$\Delta Gf^\circ = -116.657 + 1.912\times10^{-3}T\ln T - 0.130\times10^{-6}T^2 + 55.600T^{-1} - 16.200\times10^{-3}T$

550-2000 K: $\Delta Hf^\circ = -120.118 - 0.574\times10^{-3}T + 0.126\times10^{-6}T^2 + 10.900T^{-1}$

$\Delta Gf^\circ = -120.118 + 0.574\times10^{-3}T\ln T - 0.126\times10^{-6}T^2 + 5.450T^{-1} - 1.303\times10^{-3}T$

Source: Data are those estimated by Chase (24) except enthalpy of formation at 298 K converted to P(white) standard state.

$PF_3(g)$

Phosphorus Trifluoride (ideal gas)

[Formation: $P(c,l,1/4P_4(g)) + 1.5F_2(g) = PF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	14.027	65.233	65.233	0	-229.100	-223.956	164.162
300	14.066	65.320	65.233	.026	-229.106	-223.925	163.127
317.3	14.364	66.117	65.260	.272	-229.154	-223.624	154.026
317.3	14.364	66.117	65.260	.272	-229.311	-223.624	154.026
400	15.791	69.619	65.807	1.525	-229.537	-222.112	121.355
500	16.928	73.274	66.944	3.165	-229.732	-220.231	96.262
550	17.303	74.909	67.596	4.022	-229.808	-219.293	87.138
550	17.303	74.909	67.596	4.022	-232.716	-219.293	87.138
600	17.678	76.431	68.269	4.897	-232.701	-218.073	79.432
700	18.187	79.197	69.637	6.692	-232.650	-215.638	67.324
800	18.543	81.650	70.988	8.530	-232.583	-213.213	58.246
900	18.799	83.850	72.298	10.397	-232.504	-210.796	51.187
1000	18.990	85.841	73.554	12.287	-232.419	-208.390	45.543
1100	19.135	87.658	74.754	14.194	-232.328	-205.990	40.926
1200	19.247	89.328	75.901	16.113	-232.234	-203.601	37.080
1300	19.336	90.872	76.993	18.043	-232.137	-201.217	33.827
1400	19.407	92.308	78.037	19.980	-232.041	-198.844	31.041
1500	19.465	93.649	79.033	21.924	-231.944	-196.477	28.626
1600	19.513	94.906	79.985	23.873	-231.846	-194.113	26.514
1700	19.553	96.091	80.899	25.826	-231.747	-191.758	24.652
1800	19.587	97.209	81.774	27.783	-231.652	-189.407	22.997
1900	19.615	98.269	82.615	29.743	-231.555	-187.063	21.517
2000	19.640	99.276	83.423	31.706	-231.461	-184.725	20.185

Phase changes: 317.3 K, melting point of P; $\Delta H°$ = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; $\Delta H°$ = 2.908 kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 18.225 + 0.952\times10^{-3}T - 3.984\times10^{5}T^{-2}$

$H°- H°_{298} = 18.225\times10^{-3}T + 0.476\times10^{-6}T^2 + 3.984\times10^{2}T^{-1} - 6.812$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta Hf° = -230.163 + 1.664\times10^{-3}T - 2.970\times10^{-6}T^2 + 247.650T^{-1}$

$\Delta Gf° = -230.163 - 1.664\times10^{-3}T\ln T + 2.970\times10^{-6}T^2 + 123.825T^{-1} + 28.018\times10^{-3}T$

317.3-550 K: $\Delta Hf° = -229.849 - 0.829\times10^{-3}T + 0.215\times10^{-6}T^2 + 247.650T^{-1}$

$\Delta Gf° = -229.849 + 0.829\times10^{-3}T\ln T - 0.215\times10^{-6}T^2 + 123.825T^{-1} + 13.682\times10^{-3}T$

550-2000 K: $\Delta Hf° = -233.310 + 0.509\times10^{-3}T + 0.211\times10^{-6}T^2 + 147.350T^{-1}$

$\Delta Gf° = -233.310 - 0.509\times10^{-3}T\ln T - 0.211\times10^{-6}T^2 + 73.675T^{-1} + 28.580\times10^{-3}T$

Source: Data from JANAF (60) except enthalpy of formation at 298 K converted to P(white) standard state.

$PF_5(g)$

Phosphorus Pentafluoride (ideal gas)

[Formation: $P(c,l,1/4P_4(g)) + 2.5F_2(g) = PF_5(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	20.276	71.868	71.868	0	-381.100	-363.491	266.443
300	20.352	71.994	71.868	.038	-381.108	-363.383	264.721
317.3	20.934	73.151	71.906	.395	-381.175	-362.358	249.582
317.3	20.934	73.151	71.906	.395	-381.332	-362.358	249.582
400	23.718	78.342	72.712	2.252	-381.592	-357.377	195.259
500	25.941	83.891	74.405	4.743	-381.741	-351.302	153.552
550	26.679	86.407	75.382	6.064	-381.767	-348.272	138.389
550	26.679	86.407	75.382	6.064	-384.675	-348.272	138.389
600	27.416	88.760	76.400	7.416	-384.599	-344.965	125.652
700	28.421	93.066	78.479	10.211	-384.396	-338.374	105.644
800	29.128	96.910	80.548	13.090	-384.150	-331.818	90.647
900	29.640	100.372	82.561	16.030	-383.869	-325.290	78.990
1000	30.021	103.515	84.501	19.014	-383.570	-318.799	69.673
1100	30.310	106.391	86.363	22.031	-383.255	-312.337	62.055
1200	30.536	109.038	88.143	25.074	-382.928	-305.905	55.712
1300	30.714	111.490	89.846	28.137	-382.593	-299.498	50.350
1400	30.857	113.771	91.475	31.215	-382.256	-293.122	45.758
1500	30.974	115.904	93.033	34.307	-381.914	-286.768	41.781
1600	31.071	117.907	94.526	37.410	-381.568	-280.435	38.305
1700	31.151	119.793	95.957	40.521	-381.220	-274.122	35.240
1800	31.219	121.575	97.331	43.639	-380.875	-267.833	32.519
1900	31.277	123.265	98.652	46.764	-380.526	-261.561	30.086
2000	31.327	124.870	99.923	49.895	-380.181	-255.308	27.898

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to $P_4(g)$; ΔH° = 2.908 kcal/mol of P.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K:

$$Cp^\circ = 28.185 + 2.138\times10^{-3}T - 7.597\times10^{5}T^{-2}$$

$$H^\circ - H^\circ_{298} = 28.185\times10^{-3}T + 1.069\times10^{-6}T^2 + 7.597\times10^{2}T^{-1} - 11.046$$

Formation equations (kcal/mol):

298.15-317.3 K:

$$\Delta Hf^\circ = -383.508 + 3.116\times10^{-3}T - 2.551\times10^{-6}T^2 + 508.450T^{-1}$$

$$\Delta Gf^\circ = -383.508 - 3.116\times10^{-3}T\ln T + 2.551\times10^{-6}T^2 + 254.225T^{-1} + 81.268\times10^{-3}T$$

317.3-550 K:

$$\Delta Hf^\circ = -383.194 + 0.623\times10^{-3}T + 0.634\times10^{-6}T^2 + 508.450T^{-1}$$

$$\Delta Gf^\circ = -383.194 - 0.623\times10^{-3}T\ln T - 0.634\times10^{-6}T^2 + 254.225T^{-1} + 66.932\times10^{-3}T$$

550-2000 K:

$$\Delta Hf^\circ = -386.655 + 1.961\times10^{-3}T + 0.630\times10^{-6}T^2 + 408.150T^{-1}$$

$$\Delta Gf^\circ = -386.655 - 1.961\times10^{-3}T\ln T - 0.630\times10^{-6}T^2 + 204.075T^{-1} + 81.829\times10^{-3}T$$

Source: Data from JANAF (60) except enthalpy of formation at 298 K converted to P(white) standard state.

PbBr(g)

Lead Monobromide (ideal gas)

[Formation: $Pb(c,l) + 0.5Br_2(l,g) = PbBr(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.824	65.095	65.095	0	16.950	7.583	-5.559
300	8.826	65.150	65.097	.016	16.938	7.525	-5.482
332.6	8.852	66.062	65.147	.304	16.723	6.513	-4.280
332.6	8.852	66.062	65.147	.304	13.191	6.513	-4.280
400	8.905	67.701	65.443	.903	13.061	5.172	-2.826
500	8.950	69.693	66.101	1.796	12.848	3.222	-1.408
600	8.980	71.328	66.840	2.693	12.608	1.318	-.480
600.65	8.980	71.338	66.845	2.699	12.606	1.308	-.476
600.65	8.980	71.338	66.845	2.699	11.459	1.308	-.476
700	9.003	72.714	67.583	3.592	11.187	-.352	.110
800	9.023	73.917	68.301	4.493	10.917	-1.979	.541
900	9.042	74.981	68.984	5.397	10.659	-3.574	.868
1000	9.059	75.935	69.633	6.302	10.408	-5.146	1.125
1100	9.077	76.799	70.246	7.208	10.164	-6.697	1.331
1200	9.097	77.590	70.826	8.117	9.932	-8.208	1.495
1300	9.119	78.319	71.374	9.028	9.703	-9.723	1.635
1400	9.145	78.995	71.894	9.941	9.479	-11.203	1.749
1500	9.174	79.627	72.389	10.857	9.257	-12.676	1.847
1600	9.207	80.220	72.860	11.776	9.038	-14.149	1.933
1700	9.245	80.780	73.310	12.699	8.822	-15.567	2.001
1800	9.286	81.309	73.740	13.625	8.608	-16.996	2.064
1900	9.330	81.812	74.151	14.556	8.399	-18.411	2.118
2000	9.378	82.292	74.547	15.491	8.193	-19.820	2.166

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
600.65 K, melting point of Pb; ΔH° = 1.147 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.884 + 0.202\times10^{-3}T - 0.107\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.884\times10^{-3}T + 0.101\times10^{-6}T^2 + 0.107\times10^{2}T^{-1} - 2.694$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = 18.413 - 5.013\times10^{-3}T - 1.613\times10^{-6}T^2 + 52.100T^{-1}$

$\Delta Gf^\circ = 18.413 + 5.013\times10^{-3}T\ln T + 1.613\times10^{-6}T^2 + 26.050T^{-1} - 65.656\times10^{-3}T$

332.6-600.65 K: $\Delta Hf^\circ = 13.413 - 0.432\times10^{-3}T - 1.691\times10^{-6}T^2 + 36.400T^{-1}$

$\Delta Gf^\circ = 13.413 + 0.432\times10^{-3}T\ln T + 1.691\times10^{-6}T^2 + 18.200T^{-1} - 23.978\times10^{-3}T$

600.65-2000 K: $\Delta Hf^\circ = 13.065 - 2.996\times10^{-3}T + 0.287\times10^{-6}T^2 + 53.000T^{-1}$

$\Delta Gf^\circ = 13.065 + 2.996\times10^{-3}T\ln T - 0.287\times10^{-6}T^2 + 26.500T^{-1} - 38.639\times10^{-3}T$

Source: Data from Chase (27).

$PbBr_2$(c,l)
Lead Dibromide
[Formation: Pb(c,l) + Br_2(l,g) = $PbBr_2$(c,l)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.000	38.600	38.600	0	-66.600	-62.644	45.919
300	19.008	38.718	38.601	.035	-66.610	-62.619	45.617
332.6	19.154	40.686	38.711	.657	-66.784	-62.177	40.856
332.6	19.154	40.686	38.711	.657	-73.849	-62.177	40.856
400	19.457	44.240	39.350	1.956	-73.574	-59.839	32.694
500	20.179	48.653	40.783	3.935	-73.142	-56.456	24.677
600	21.240	52.421	42.416	6.003	-72.655	-53.165	19.365
600.65	21.249	52.444	42.427	6.017	-72.651	-53.142	19.336
600.65	21.249	52.444	42.427	6.017	-73.798	-53.142	19.336
644	21.822	53.944	43.152	6.950	-73.568	-51.659	17.531
644	26.800	60.062	43.152	10.890	-69.628	-51.659	17.531
700	26.800	62.296	44.595	12.391	-69.033	-50.123	15.649
800	26.800	65.875	47.036	15.071	-67.972	-47.491	12.974
900	26.800	69.031	49.308	17.751	-66.903	-44.994	10.926
1000	26.800	71.855	51.424	20.431	-65.829	-42.622	9.315
1100	26.800	74.409	53.399	23.111	-64.750	-40.360	8.019
1200	26.800	76.741	55.248	25.791	-63.663	-38.179	6.953

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
600.65 K, melting point of Pb; ΔH° = 1.147 kcal/mol.
644 K, melting point of $PbBr_2$; ΔH° = 3.940 kcal/mol.
1202 K, calculated boiling point to $PbBr_2$(g); ΔH° = 28.3 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-644 K: $Cp° = 14.025 + 11.312\times10^{-3}T + 1.424\times10^{5}T^{-2}$
$H°- H°_{298} = 14.025\times10^{-3}T + 5.656\times10^{-6}T^2 - 1.424\times10^{2}T^{-1} - 4.207$
644-1200 K: $Cp° = 26.800$
$H°- H°_{298} = 26.800\times10^{-3}T - 6.369$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -63.958 - 8.917\times10^{-3}T + 3.992\times10^{-6}T^2 - 101.000T^{-1}$
$\Delta Gf° = -63.958 + 8.917\times10^{-3}T\ln T - 3.992\times10^{-6}T^2 - 50.500T^{-1} - 44.641\times10^{-3}T$
332.6-600.65 K: $\Delta Hf° = -73.958 + 0.244\times10^{-3}T + 3.837\times10^{-6}T^2 - 132.400T^{-1}$
$\Delta Gf° = -73.958 - 0.244\times10^{-3}T\ln T - 3.837\times10^{-6}T^2 - 66.200T^{-1} + 38.714\times10^{-3}T$
600.65-644 K: $\Delta Hf° = -74.306 - 2.320\times10^{-3}T + 5.814\times10^{-6}T^2 - 115.800T^{-1}$
$\Delta Gf° = -74.306 + 2.320\times10^{-3}T\ln T - 5.814\times10^{-6}T^2 - 57.900T^{-1} + 24.053\times10^{-3}T$
644-1200 K: $\Delta Hf° = -76.468 + 10.455\times10^{-3}T + 0.158\times10^{-6}T^2 + 26.600T^{-1}$
$\Delta Gf° = -76.468 - 10.455\times10^{-3}T\ln T - 0.158\times10^{-6}T^2 + 13.300T^{-1} + 106.222\times10^{-3}T$

Sources: Enthalpy of formation at 298 K and entropy at 298 K from Wagman (252). Low-temperature heat capacities from Latimer (141). High-temperature data based on Linsey (144).

$PbBr_2(g)$

Lead Dibromide (ideal gas)

[Formation: $Pb(c,1) + Br_2(l,g) = PbBr_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	13.603	81.089	81.089	0	-24.950	-33.662	24.675
300	13.607	81.173	81.090	.025	-24.970	-33.716	24.561
332.6	13.649	82.579	81.168	.469	-25.322	-34.648	22.767
332.6	13.649	82.579	81.168	.469	-32.387	-34.648	22.767
400	13.736	85.108	81.626	1.393	-32.487	-35.099	19.177
500	13.798	88.180	82.640	2.770	-32.657	-35.735	15.620
600	13.832	90.699	83.779	4.152	-32.856	-36.333	13.234
600.65	13.832	90.714	83.786	4.161	-32.857	-36.335	13.220
600.65	13.832	90.714	83.786	4.161	-34.004	-36.335	13.220
700	13.852	92.833	84.924	5.536	-34.238	-36.704	11.459
800	13.866	94.684	86.032	6.922	-34.471	-37.037	10.118
900	13.875	96.317	87.085	8.309	-34.695	-37.344	9.068
1000	13.882	97.780	88.083	9.697	-34.913	-37.631	8.224
1100	13.887	99.103	89.025	11.086	-35.125	-37.898	7.530
1200	13.890	100.312	89.917	12.474	-35.330	-38.131	6.944
1300	13.893	101.423	90.758	13.864	-35.532	-38.367	6.450
1400	13.896	102.453	91.558	15.253	-35.733	-38.574	6.022
1500	13.898	103.412	92.317	16.643	-35.935	-38.773	5.649
1600	13.899	104.309	93.038	18.033	-36.138	-38.973	5.323
1700	13.900	105.152	93.727	19.423	-36.342	-39.120	5.029
1800	13.901	105.946	94.383	20.813	-36.547	-39.278	4.769
1900	13.902	106.698	95.012	22.203	-36.753	-39.422	4.535
2000	13.903	107.411	95.615	23.593	-36.961	-39.561	4.323

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
600.65 K, melting point of Pb; $\Delta H°$ = 1.147 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.902 + 0.006\times10^{-3}T - 0.267\times10^{5}T^{-2}$

$H°- H°_{298} = 13.902\times10^{-3}T + 0.003\times10^{-6}T^{2} + 0.267\times10^{2}T^{-1} - 4.235$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -22.335 - 9.040\times10^{-3}T - 1.661\times10^{-6}T^{2} + 68.100T^{-1}$

$\Delta Gf° = -22.335 + 9.040\times10^{-3}T\ln T + 1.661\times10^{-6}T^{2} + 34.050T^{-1} - 90.374\times10^{-3}T$

332.6-600.65 K: $\Delta Hf° = -32.336 + 0.121\times10^{-3}T - 1.816\times10^{-6}T^{2} + 36.700T^{-1}$

$\Delta Gf° = -32.336 - 0.121\times10^{-3}T\ln T + 1.816\times10^{-6}T^{2} + 18.350T^{-1} - 7.019\times10^{-3}T$

600.65-2000 K: $\Delta Hf° = -32.684 - 2.443\times10^{-3}T + 0.161\times10^{-6}T^{2} + 53.300T^{-1}$

$\Delta Gf° = -32.684 + 2.443\times10^{-3}T\ln T - 0.161\times10^{-6}T^{2} + 26.650T^{-1} - 21.680\times10^{-3}T$

Source: Data from Chase (27).

$PbBr_4(g)$
Lead Tetrabromide (ideal gas)
[Formation: $Pb(c,l) + 2Br_2(l,g) = PbBr_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	25.007	101.837	101.837	0	-109.073	-113.125	82.921
300	25.017	101.992	101.839	.046	-109.105	-113.149	82.428
332.6	25.130	104.579	101.983	.863	-109.672	-113.560	74.619
332.6	25.130	104.579	101.983	.863	-123.802	-113.560	74.619
400	25.363	109.243	102.823	2.568	-123.710	-111.498	60.919
500	25.529	114.922	104.696	5.113	-123.594	-108.461	47.408
600	25.621	119.586	106.801	7.671	-123.505	-105.444	38.407
600.65	25.621	119.614	106.815	7.688	-123.504	-105.422	38.358
600.65	25.621	119.614	106.815	7.688	-124.651	-105.422	38.358
700	25.677	123.540	108.917	10.236	-124.599	-102.248	31.923
800	25.713	126.971	110.964	12.806	-124.543	-99.054	27.060
900	25.738	130.001	112.914	15.378	-124.481	-95.873	23.281
1000	25.756	132.714	114.761	17.953	-124.412	-92.702	20.260
1100	25.769	135.169	116.506	20.529	-124.339	-89.541	17.790
1200	25.780	137.412	118.156	23.107	-124.257	-86.368	15.730
1300	25.787	139.476	119.718	25.685	-124.176	-83.229	13.992
1400	25.794	141.387	121.198	28.264	-124.093	-80.076	12.500
1500	25.799	143.167	122.604	30.844	-124.013	-76.939	11.210
1600	25.803	144.832	123.942	33.424	-123.935	-73.820	10.083
1700	25.806	146.396	125.217	36.005	-123.858	-70.665	9.084
1800	25.809	147.871	126.435	38.585	-123.784	-67.539	8.200
1900	25.812	149.267	127.601	41.166	-123.711	-64.414	7.409
2000	25.814	150.591	128.717	43.748	-123.641	-61.299	6.698

*Data estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
600.65 K, melting point of Pb; ΔH° = 1.147 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 25.813 + 0.012\times10^{-3}T - 0.720\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.813\times10^{-3}T + 0.006\times10^{-6}T^2 + 0.720\times10^{2}T^{-1} - 7.938$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -104.777 - 15.220\times10^{-3}T - 1.558\times10^{-6}T^2 + 113.400T^{-1}$

$\Delta Gf^\circ = -104.777 + 15.220\times10^{-3}T\ln T + 1.558\times10^{-6}T^2 + 56.700T^{-1} - 115.818\times10^{-3}T$

332.6-600.65 K: $\Delta Hf^\circ = -124.778 + 3.102\times10^{-3}T - 1.868\times10^{-6}T^2 + 50.600T^{-1}$

$\Delta Gf^\circ = -124.778 - 3.102\times10^{-3}T\ln T + 1.868\times10^{-6}T^2 + 25.300T^{-1} + 50.893\times10^{-3}T$

600.65-2000 K: $\Delta Hf^\circ = -125.126 + 0.538\times10^{-3}T + 0.109\times10^{-6}T^2 + 67.200T^{-1}$

$\Delta Gf^\circ = -125.126 - 0.538\times10^{-3}T\ln T - 0.109\times10^{-6}T^2 + 33.600T^{-1} + 36.232\times10^{-3}T$

Source: Data are estimates from Chase (27).

PbCl(g)
Lead Monochloride (ideal gas)
[Formation: $Pb(c,l) + 0.5Cl_2(g) = PbCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.660	62.022	62.022	0	3.600	-2.329	1.707
300	8.664	62.075	62.022	.016	3.596	-2.366	1.724
400	8.805	64.589	62.364	.890	3.412	-4.326	2.364
500	8.881	66.563	63.013	1.775	3.206	-6.238	2.727
600	8.929	68.187	63.744	2.666	2.969	-8.107	2.953
600.65	8.929	68.197	63.748	2.672	2.968	-8.117	2.953
600.65	8.929	68.197	63.748	2.672	1.821	-8.117	2.953
700	8.963	69.566	64.480	3.560	1.551	-9.742	3.041
800	8.989	70.765	65.192	4.458	1.283	-11.334	3.096
900	9.012	71.825	65.872	5.358	1.025	-12.894	3.131
1000	9.032	72.775	66.515	6.260	.775	-14.432	3.154
1100	9.052	73.637	67.124	7.164	.531	-15.948	3.168
1200	9.073	74.425	67.699	8.071	.298	-17.422	3.173
1300	9.096	75.152	68.245	8.979	.068	-18.903	3.178
1400	9.122	75.827	68.763	9.890	-.157	-20.349	3.177
1500	9.151	76.458	69.256	10.803	-.381	-21.788	3.175
1600	9.185	77.049	69.724	11.720	-.602	-23.225	3.172
1700	9.222	77.607	70.172	12.640	-.821	-24.606	3.163
1800	9.263	78.136	70.600	13.565	-1.035	-26.002	3.157
1900	9.307	78.638	71.010	14.493	-1.247	-27.382	3.150
2000	9.354	79.116	71.403	15.426	-1.456	-28.753	3.142

Phase change: 600.65 K, melting point of Pb; ΔH° = 1.147 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.869 + 0.200\times10^{-3}T - 0.239\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.869\times10^{-3}T + 0.100\times10^{-6}T^2 + 0.239\times10^{2}T^{-1} - 2.733$

Formation equations (kcal/mol):

298.15-600.65 K: $\Delta Hf^\circ = 3.765 - 0.395\times10^{-3}T - 1.708\times10^{-6}T^2 + 31.150T^{-1}$

$\Delta Gf^\circ = 3.765 + 0.395\times10^{-3}T\ln T + 1.708\times10^{-6}T^2 + 15.575T^{-1} - 23.379\times10^{-3}T$

600.65-2000 K: $\Delta Hf^\circ = 3.417 - 2.959\times10^{-3}T + 0.269\times10^{-6}T^2 + 47.750T^{-1}$

$\Delta Gf^\circ = 3.417 + 2.959\times10^{-3}T\ln T - 0.269\times10^{-6}T^2 + 23.875T^{-1} - 38.040\times10^{-3}T$

Source: Data from Chase (27).

$PbCl_2(c,l)$
Lead Dichloride
[Formation: $Pb(c,l) + Cl_2(g) = PbCl_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	18.380	32.500	32.500	0	-85.900	-75.083	55.037
300	18.389	32.614	32.501	.034	-85.893	-75.016	54.649
400	18.983	37.981	33.229	1.901	-85.499	-71.449	39.038
500	19.684	42.291	34.623	3.834	-85.084	-67.985	29.716
600	20.437	45.946	36.213	5.840	-84.640	-64.608	23.533
600.65	20.442	45.968	36.223	5.853	-84.636	-64.584	23.499
600.65	20.442	45.968	36.223	5.853	-85.783	-64.584	23.499
700	21.226	49.155	37.836	7.923	-85.308	-61.115	19.081
771	21.803	51.233	38.976	9.450	-84.926	-58.679	16.633
771	26.050	58.016	38.976	14.680	-79.696	-58.679	16.633
800	26.738	58.991	39.685	15.445	-79.396	-57.894	15.816
900	29.110	62.277	42.013	18.238	-78.205	-55.273	13.422
1000	31.482	65.467	44.199	21.268	-76.775	-52.804	11.540
1100	33.855	68.579	46.275	24.534	-75.105	-50.494	10.032
1200	36.227	71.626	48.261	28.038	-73.191	-48.327	8.801

*Heat capacity at 298 K estimated.

Phase changes: 600.65 K, melting point of Pb; ΔH° = 1.147 kcal/mol.
771 K, melting point of $PbCl_2$; ΔH° = 5.230 kcal/mol.
1236 K, calculated boiling point of $PbCl_2$ to monomer; ΔH° = 28 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-771 K: $Cp^\circ = 15.444 + 8.122\times10^{-3}T + 0.457\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 15.444\times10^{-3}T + 4.061\times10^{-6}T^2 - 0.457\times10^{2}T^{-1} - 4.812$

771-1200 K: $Cp^\circ = 7.933 + 23.594\times10^{-3}T - 0.442\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 7.933\times10^{-3}T + 11.797\times10^{-6}T^2 + 0.442\times10^{2}T^{-1} + 1.494$

Formation equations (kcal/mol):

298.15-600.65 K: $\Delta Hf^\circ = -86.379 + 1.766\times10^{-3}T + 2.209\times10^{-6}T^2 - 72.600T^{-1}$

$\Delta Gf^\circ = -86.379 - 1.766\times10^{-3}T\ln T - 2.209\times10^{-6}T^2 - 36.300T^{-1} + 49.017\times10^{-3}T$

600.65-771 K: $\Delta Hf^\circ = -86.727 - 0.798\times10^{-3}T + 4.186\times10^{-6}T^2 - 56.000T^{-1}$

$\Delta Gf^\circ = -86.727 + 0.798\times10^{-3}T\ln T - 4.186\times10^{-6}T^2 - 28.000T^{-1} + 34.356\times10^{-3}T$

771-1200 K: $\Delta Hf^\circ = -80.421 - 8.309\times10^{-3}T + 11.922\times10^{-6}T^2 + 33.900T^{-1}$

$\Delta Gf^\circ = -80.421 + 8.309\times10^{-3}T\ln T - 11.922\times10^{-6}T^2 + 16.950T^{-1} - 17.865\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Entropy at 298 K from Kelley (118). Heat capacity at 298 K estimated. High-temperature data based on Linsey (144).

$PbCl_2(g)$

Lead Dichloride (ideal gas)

[Formation: $Pb(c,l) + Cl_2(g) = PbCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	13.189	75.787	75.787	0	-41.600	-43.689	32.025
300	13.197	75.868	75.788	.024	-41.603	-43.702	31.837
400	13.490	79.710	76.308	1.361	-41.739	-44.381	24.248
500	13.635	82.738	77.302	2.718	-41.900	-45.024	19.680
600	13.717	85.231	78.421	4.086	-42.094	-45.633	16.622
600.65	13.717	85.246	78.428	4.095	-42.095	-45.634	16.604
600.65	13.717	85.246	78.428	4.095	-43.242	-45.634	16.604
700	13.767	87.350	79.550	5.460	-43.471	-46.015	14.366
800	13.800	89.191	80.644	6.838	-43.703	-46.361	12.665
900	13.823	90.817	81.684	8.220	-43.923	-46.677	11.335
1000	13.839	92.275	82.672	9.603	-44.140	-46.977	10.267
1100	13.851	93.594	83.606	10.987	-44.352	-47.257	9.389
1200	13.861	94.800	84.489	12.373	-44.556	-47.501	8.651
1300	13.868	95.910	85.326	13.759	-44.759	-47.752	8.028
1400	13.874	96.938	86.119	15.147	-44.959	-47.969	7.488
1500	13.878	97.895	86.872	16.534	-45.162	-48.180	7.020
1600	13.882	98.791	87.590	17.922	-45.366	-48.393	6.610
1700	13.885	99.633	88.274	19.311	-45.570	-48.548	6.241
1800	13.888	100.426	88.927	20.699	-45.777	-48.720	5.915
1900	13.890	101.177	89.552	22.088	-45.984	-48.876	5.622
2000	13.893	101.890	90.151	23.477	-46.194	-49.026	5.357

Phase change: 600.65 K, melting point of Pb; ΔH° = 1.147 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.874 + 0.022\times10^{-3}T - 0.614\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.874\times10^{-3}T + 0.011\times10^{-6}T^2 + 0.614\times10^{2}T^{-1} - 4.343$

Formation equations (kcal/mol):

298.15-600.65 K: $\Delta Hf^\circ = -41.610 + 0.196\times10^{-3}T - 1.841\times10^{-6}T^2 + 34.500T^{-1}$

$\Delta Gf^\circ = -41.610 - 0.196\times10^{-3}T\ln T + 1.841\times10^{-6}T^2 + 17.250T^{-1} - 6.598\times10^{-3}T$

600.65-2000 K: $\Delta Hf^\circ = -41.958 - 2.368\times10^{-3}T + 0.136\times10^{-6}T^2 + 51.100T^{-1}$

$\Delta Gf^\circ = -41.958 + 2.368\times10^{-3}T\ln T - 0.136\times10^{-6}T^2 + 25.550T^{-1} - 21.259\times10^{-3}T$

Source: Data from Chase (27).

$PbCl_4(g)$

Lead Tetrachloride (ideal gas)

[Formation: $Pb(c,l) + 2Cl_2(g) = PbCl_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	24.028	91.191	91.191	0	-132.028	-122.821	90.029
300	24.048	91.340	91.193	.044	-132.026	-122.765	89.433
400	24.775	98.371	92.146	2.490	-131.883	-119.699	65.400
500	25.139	103.943	93.967	4.988	-131.756	-116.668	50.995
600	25.345	108.546	96.024	7.513	-131.662	-113.662	41.401
600.65	25.346	108.573	96.038	7.529	-131.661	-113.640	41.348
600.65	25.346	108.573	96.038	7.529	-132.808	-113.640	41.348
700	25.471	112.463	98.100	10.054	-132.750	-110.477	34.492
800	25.555	115.870	100.113	12.606	-132.694	-107.297	29.312
900	25.612	118.884	102.035	15.164	-132.628	-104.125	25.285
1000	25.654	121.584	103.856	17.728	-132.558	-100.966	22.066
1100	25.685	124.031	105.581	20.295	-132.484	-97.818	19.434
1200	25.708	126.267	107.214	22.864	-132.405	-94.659	17.240
1300	25.727	128.325	108.759	25.436	-132.324	-91.529	15.387
1400	25.741	130.232	110.225	28.010	-132.242	-88.388	13.798
1500	25.753	132.009	111.620	30.584	-132.164	-85.264	12.423
1600	25.763	133.671	112.946	33.160	-132.088	-82.157	11.222
1700	25.771	135.233	114.211	35.737	-132.013	-79.009	10.157
1800	25.777	136.707	115.421	38.314	-131.942	-75.899	9.215
1900	25.783	138.100	116.578	40.892	-131.872	-72.782	8.372
2000	25.788	139.423	117.688	43.471	-131.807	-69.677	7.614

Phase change: 600.65 K, melting point of Pb; $\Delta H° = 1.147$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 25.722 + 0.070\times10^{-3}T - 1.524\times10^{5}T^{-2}$

$H°- H°_{298} = 25.722\times10^{-3}T + 0.035\times10^{-6}T^2 + 1.524\times10^{2}T^{-1} - 8.183$

Formation equations (kcal/mol):

298.15-600.65 K: $\Delta Hf° = -133.010 + 3.217\times10^{-3}T - 1.905\times10^{-6}T^2 + 57.200T^{-1}$

$\Delta Gf° = -133.010 - 3.217\times10^{-3}T\ln T + 1.905\times10^{-6}T^2 + 28.600T^{-1} + 51.611\times10^{-3}T$

600.65-2000 K: $\Delta Hf° = -133.357 + 0.653\times10^{-3}T + 0.072\times10^{-6}T^2 + 73.800T^{-1}$

$\Delta Gf° = -133.357 - 0.653\times10^{-3}T\ln T - 0.072\times10^{-6}T^2 + 36.900T^{-1} + 36.950\times10^{-3}T$

Source: Data from Chase (27).

PbF(g)

Lead Monofluoride (ideal gas)

[Formation: $Pb(c,l) + 0.5F_2(g) = PbF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.221	59.714	59.714	0	-19.184	-25.148	18.434
300	8.229	59.765	59.715	.015	-19.188	-25.185	18.347
400	8.514	62.175	60.040	.854	-19.376	-27.154	14.836
500	8.675	64.094	60.666	1.714	-19.583	-29.077	12.709
600	8.775	65.685	61.373	2.587	-19.819	-30.956	11.276
600.65	8.775	65.694	61.378	2.593	-19.820	-30.966	11.267
600.65	8.775	65.694	61.378	2.593	-20.967	-30.966	11.267
700	8.843	67.043	62.089	3.468	-21.235	-32.600	10.178
800	8.891	68.227	62.783	4.355	-21.503	-34.203	9.344
900	8.929	69.277	63.448	5.246	-21.759	-35.774	8.687
1000	8.959	70.219	64.079	6.140	-22.011	-37.323	8.157
1100	8.987	71.075	64.677	7.038	-22.255	-38.848	7.718
1200	9.013	71.858	65.243	7.938	-22.491	-40.335	7.346
1300	9.040	72.580	65.780	8.840	-22.723	-41.825	7.031
1400	9.069	73.251	66.290	9.746	-22.951	-43.282	6.757
1500	9.100	73.878	66.775	10.654	-23.179	-44.730	6.517
1600	9.135	74.466	67.237	11.566	-23.404	-46.176	6.307
1700	9.173	75.021	67.679	12.481	-23.627	-47.567	6.115
1800	9.214	75.546	68.102	13.400	-23.848	-48.970	5.946
1900	9.258	76.046	68.507	14.324	-24.064	-50.360	5.793
2000	9.305	76.522	68.896	15.252	-24.279	-51.741	5.654

Phase change: 600.65 K, melting point of Pb; ΔH° = 1.147 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.791 + 0.228\times10^{-3}T - 0.567\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.791\times10^{-3}T + 0.114\times10^{-6}T^2 + 0.567\times10^{2}T^{-1} - 2.821$

Formation equations (kcal/mol):

298.15-600.65 K: $\Delta Hf^\circ = -19.096 - 0.314\times10^{-3}T - 1.737\times10^{-6}T^2 + 47.850T^{-1}$

$\Delta Gf^\circ = -19.096 + 0.314\times10^{-3}T\ln T + 1.737\times10^{-6}T^2 + 23.925T^{-1} - 22.872\times10^{-3}T$

600.65-2000 K: $\Delta Hf^\circ = -19.444 - 2.878\times10^{-3}T + 0.240\times10^{-6}T^2 + 64.450T^{-1}$

$\Delta Gf^\circ = -19.444 + 2.878\times10^{-3}T\ln T - 0.240\times10^{-6}T^2 + 32.225T^{-1} - 37.533\times10^{-3}T$

Source: Data from Chase (27).

PbF_2(c,l)
Lead Difluoride
[Formation: Pb(c,l) + F_2(g) = PbF_2(c,l)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	17.034	26.400	26.400	0	-158.700	-147.510	108.126
300	17.058	26.505	26.400	.032	-158.694	-147.440	107.408
400	18.098	31.564	27.084	1.792	-158.346	-143.740	78.535
500	18.919	35.692	28.404	3.644	-157.963	-140.132	61.251
583	19.531	38.644	29.656	5.240	-157.628	-137.201	51.432
583	21.076	39.279	29.656	5.610	-157.258	-137.201	51.432
600	21.917	39.896	29.938	5.975	-157.155	-136.618	49.762
600.65	21.986	39.920	29.948	5.989	-157.150	-136.593	49.700
600.65	21.986	39.920	29.948	5.989	-158.297	-136.593	49.700
700	32.492	43.924	31.637	8.601	-157.250	-133.073	41.547
745	41.827	46.217	32.445	10.260	-156.303	-131.546	38.589
800	25.723	48.143	33.461	11.746	-155.691	-129.740	35.443
900	22.688	50.973	35.255	14.146	-154.874	-126.546	30.729
1000	22.081	53.311	36.947	16.364	-154.242	-123.438	26.977
1100	23.903	55.482	38.534	18.643	-153.548	-120.396	23.920
1103	23.995	55.547	38.580	18.715	-153.524	-120.305	23.837
1103	26.100	58.779	38.580	22.280	-149.959	-120.305	23.837
1200	26.100	60.979	40.302	24.812	-148.960	-117.729	21.441
1300	26.100	63.068	41.974	27.422	-147.932	-115.180	19.363
1400*	26.100	65.002	43.551	30.032	-146.906	-112.696	17.592

*PbF_2 disproportionates on vaporizing.

Phase changes: 583 K, orthorhombic-cubic transition point of PbF_2; ΔH° = 0.370 kcal/mol. Cubic form metastable below 583 K.
600.65 K, melting point of Pb; ΔH° = 1.147 kcal/mol.
745 K, second order transition point of PbF_2; ΔH° = 0 kcal/mol.
1103 K, melting point of PbF_2; ΔH° = 3.565 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-583 K: $Cp° = 16.088 + 6.330\times10^{-3}T - 0.839\times10^{5}T^{-2}$
$H°- H°_{298} = 16.088\times10^{-3}T + 3.165\times10^{-6}T^{2} + 0.839\times10^{2}T^{-1} - 5.359$

583-745 K: $Cp° = -37.532 + 99.752\times10^{-3}T$
$H°- H°_{298} = -37.532\times10^{-3}T + 49.876\times10^{-6}T^{2} + 10.539$

745-1103 K: $Cp° = 36.853 - 14.326\times10^{-3}T + 0.020\times10^{5}T^{-2}$
$H°- H°_{298} = 36.853\times10^{-3}T - 7.163\times10^{-6}T^{2} - 0.020\times10^{2}T^{-1} - 13.217$

1103-1400 K: $Cp° = 26.100$
$H°- H°_{298} = 26.100\times10^{-3}T - 6.508$

PbF_2(c,l) - Continued

Formation equations (kcal/mol):

298.15-583 K: $\Delta Hf^\circ = -159.706 + 2.729\times10^{-3}T + 1.227\times10^{-6}T^2 + 24.800T^{-1}$

$\Delta Gf^\circ = -159.706 - 2.729\times10^{-3}T\ln T - 1.227\times10^{-6}T^2 + 12.400T^{-1} + 56.682\times10^{-3}T$

583-600.65 K: $\Delta Hf^\circ = -143.808 - 50.891\times10^{-3}T + 47.938\times10^{-6}T^2 - 59.100T^{-1}$

$\Delta Gf^\circ = -143.808 + 50.891\times10^{-3}T\ln T - 47.938\times10^{-6}T^2 - 29.550T^{-1} - 284.693\times10^{-3}T$

600.65-745 K: $\Delta Hf^\circ = -144.156 - 53.455\times10^{-3}T + 49.915\times10^{-6}T^2 - 42.500T^{-1}$

$\Delta Gf^\circ = -144.156 + 53.455\times10^{-3}T\ln T - 49.915\times10^{-6}T^2 - 21.250T^{-1} - 299.354\times10^{-3}T$

745-1103 K: $\Delta Hf^\circ = -167.912 + 20.930\times10^{-3}T - 7.124\times10^{-6}T^2 - 44.500T^{-1}$

$\Delta Gf^\circ = -167.912 - 20.930\times10^{-3}T\ln T + 7.124\times10^{-6}T^2 - 22.250T^{-1} + 181.977\times10^{-3}T$

1103-1400 K: $\Delta Hf^\circ = -161.203 + 10.177\times10^{-3}T + 0.039\times10^{-6}T^2 - 42.500T^{-1}$

$\Delta Gf^\circ = -161.203 - 10.177\times10^{-3}T\ln T - 0.039\times10^{-6}T^2 - 21.250T^{-1} + 108.461\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (252). High-temperature data based on Linsey (144). Temperature of transition at 745 K from Rimai (198).

$PbF_2(g)$

Lead Difluoride (ideal gas)

[Formation: $Pb(c,l) + F_2(g) = PbF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.177	69.928	69.928	0	-104.000	-105.787	77.543
300	12.193	70.003	69.928	.023	-104.003	-105.798	77.073
400	12.823	73.607	70.415	1.277	-104.161	-106.372	58.118
500	13.173	76.509	71.353	2.578	-104.329	-106.907	46.728
600	13.381	78.931	72.419	3.907	-104.523	-107.407	39.122
600.65	13.382	78.945	72.426	3.916	-104.524	-107.407	39.080
600.65	13.382	78.945	72.426	3.916	-105.671	-107.407	39.080
700	13.514	81.004	73.501	5.252	-105.899	-107.678	33.618
800	13.603	82.815	74.555	6.608	-106.129	-107.915	29.481
900	13.665	84.421	75.564	7.971	-106.349	-108.124	26.256
1000	13.710	85.863	76.523	9.340	-106.566	-108.314	23.672
1100	13.744	87.171	77.432	10.713	-106.778	-108.484	21.554
1200	13.770	88.368	78.294	12.089	-106.983	-108.619	19.782
1300	13.791	89.471	79.112	13.467	-107.187	-108.759	18.284
1400	13.807	90.494	79.889	14.847	-107.391	-108.869	16.995
1500	13.820	91.447	80.628	16.228	-107.597	-108.971	15.877
1600	13.831	92.339	81.332	17.611	-107.804	-109.073	14.898
1700	13.840	93.178	82.005	18.994	-108.013	-109.120	14.028
1800	13.847	93.969	82.647	20.379	-108.224	-109.180	13.256
1900	13.854	94.718	83.263	21.764	-108.436	-109.226	12.564
2000	13.859	95.429	83.854	23.149	-108.652	-109.266	11.940

Phase change: 600.65 K, melting point of Pb; ΔH° = 1.147 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.652 + 0.162\times10^{-3}T - 1.354\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.652\times10^{-3}T + 0.081\times10^{-6}T^2 + 1.354\times10^{2}T^{-1} - 4.532$

Formation equations (kcal/mol):

298.15-600.65 K: $\Delta Hf^\circ = -104.178 + 0.293\times10^{-3}T - 1.857\times10^{-6}T^2 + 76.300T^{-1}$

$\Delta Gf^\circ = -104.178 - 0.293\times10^{-3}T\ln T + 1.857\times10^{-6}T^2 + 38.150T^{-1} - 4.711\times10^{-3}T$

600.65-2000 K: $\Delta Hf^\circ = -104.526 - 2.271\times10^{-3}T + 0.120\times10^{-6}T^2 + 92.900T^{-1}$

$\Delta Gf^\circ = -104.526 + 2.271\times10^{-3}T\ln T - 0.120\times10^{-6}T^2 + 46.450T^{-1} - 19.372\times10^{-3}T$

Source: Data from Chase (27).

$PbF_4(g)$

Lead Tetrafluoride (ideal gas)

[Formation: $Pb(c,l) + 2F_2(g) = PbF_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	21.734	79.706	79.706	0	-270.900	-261.159	191.433
300	21.771	79.841	79.708	.040	-270.900	-261.100	190.209
400	23.249	86.328	80.581	2.299	-270.822	-257.841	140.876
500	24.075	91.613	82.275	4.669	-270.725	-254.608	111.288
600	24.570	96.050	84.212	7.103	-270.644	-251.396	91.570
600.65	24.572	96.077	84.224	7.119	-270.643	-251.373	91.462
600.65	24.572	96.077	84.224	7.119	-271.790	-251.373	91.462
700	24.885	99.862	86.181	9.577	-271.739	-248.001	77.428
800	25.097	103.200	88.104	12.077	-271.687	-244.612	66.824
900	25.246	106.165	89.949	14.594	-271.624	-241.228	58.577
1000	25.354	108.831	91.707	17.124	-271.560	-237.861	51.984
1100	25.435	111.251	93.375	19.664	-271.491	-234.499	46.590
1200	25.497	113.467	94.958	22.211	-271.416	-231.128	42.094
1300	25.546	115.510	96.462	24.763	-271.341	-227.786	38.294
1400	25.585	117.405	97.891	27.320	-271.268	-224.437	35.036
1500	25.617	119.171	99.251	29.880	-271.198	-221.096	32.213
1600	25.643	120.825	100.548	32.443	-271.131	-217.776	29.746
1700	25.664	122.381	101.788	35.008	-271.066	-214.417	27.565
1800	25.682	123.848	102.972	37.576	-271.006	-211.088	25.629
1900	25.698	125.237	104.108	40.145	-270.947	-207.759	23.897
2000	25.711	126.555	105.198	42.715	-270.895	-204.437	22.340

*Data except enthalpy of formation at 298 K estimated.

Phase change: 600.65 K, melting point of Pb; ΔH° = 1.147 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 25.199 + 0.396\times10^{-3}T - 3.185\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.199\times10^{-3}T + 0.198\times10^{-6}T^2 + 3.185\times10^{2}T^{-1} - 8.599$

Formation equations (kcal/mol):

298.15-600.65 K: $\Delta Hf^\circ = -272.256 + 3.332\times10^{-3}T - 1.914\times10^{-6}T^2 + 158.900T^{-1}$

$\Delta Gf^\circ = -272.256 - 3.332\times10^{-3}T\ln T + 1.914\times10^{-6}T^2 + 79.450T^{-1} + 54.739\times10^{-3}T$

600.65-2000 K: $\Delta Hf^\circ = -272.604 + 0.768\times10^{-3}T + 0.063\times10^{-6}T^2 + 175.500T^{-1}$

$\Delta Gf^\circ = -272.604 - 0.768\times10^{-3}T\ln T - 0.063\times10^{-6}T^2 + 87.750T^{-1} + 40.078\times10^{-3}T$

Source: Data from Chase (27). All are estimates except enthalpy of formation at 298 K.

PbI(g)

Lead Monoiodide (ideal gas)

[Formation: $Pb(c,l) + 0.5I_2(c,l,g) = PbI(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.880	66.917	66.917	0	25.750	14.555	-10.669
300	8.881	66.972	66.919	.016	25.742	14.485	-10.552
386.8	8.927	69.235	67.195	.789	25.354	11.278	-6.372
386.8	8.927	69.235	67.195	.789	23.500	11.278	-6.372
400	8.934	69.535	67.268	.907	23.404	10.862	-5.935
458.4	8.952	70.754	67.634	1.430	22.979	9.062	-4.320
458.4	8.952	70.754	67.634	1.430	17.969	9.062	-4.320
500	8.965	71.532	67.926	1.803	17.876	8.258	-3.610
600	8.987	73.168	68.668	2.700	17.632	6.355	-2.315
600.65	8.987	73.178	68.673	2.706	17.630	6.345	-2.309
600.65	8.987	73.178	68.673	2.706	16.483	6.345	-2.309
700	9.005	74.555	69.412	3.600	16.209	4.688	-1.464
800	9.020	75.758	70.132	4.501	15.935	3.064	-.837
900	9.035	76.822	70.818	5.404	15.674	1.471	-.357
1000	9.050	77.774	71.466	6.308	15.420	-.097	.021
1100	9.066	78.638	72.080	7.214	15.174	-1.644	.327
1200	9.083	79.427	72.660	8.121	14.936	-3.150	.574
1300	9.103	80.155	73.209	9.030	14.703	-4.661	.784
1400	9.127	80.831	73.730	9.942	14.476	-6.138	.958
1500	9.154	81.461	74.224	10.856	14.249	-7.605	1.108
1600	9.186	82.053	74.695	11.773	14.025	-9.073	1.239
1700	9.221	82.611	75.145	12.693	13.803	-10.484	1.348
1800	9.261	83.139	75.574	13.617	13.584	-11.908	1.446
1900	9.303	83.641	75.986	14.545	13.369	-13.318	1.532
2000	9.349	84.119	76.380	15.478	13.158	-14.718	1.608

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
600.65 K, melting point of Pb; ΔH° = 1.147 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.894 + 0.178\times10^{-3}T - 0.060\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.894\times10^{-3}T + 0.089\times10^{-6}T^2 + 0.060\times10^{2}T^{-1} - 2.680$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = 26.520 - 2.395\times10^{-3}T - 2.421\times10^{-6}T^2 + 47.400T^{-1}$

$\Delta Gf^\circ = 26.520 + 2.395\times10^{-3}T\ln T + 2.421\times10^{-6}T^2 + 23.700T^{-1} - 54.769\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = 25.793 - 5.598\times10^{-3}T - 1.675\times10^{-6}T^2 + 47.400T^{-1}$

$\Delta Gf^\circ = 25.793 + 5.598\times10^{-3}T\ln T + 1.675\times10^{-6}T^2 + 23.700T^{-1} - 71.677\times10^{-3}T$

458.4-600.65 K: $\Delta Hf^\circ = 18.436 - 0.428\times10^{-3}T - 1.709\times10^{-6}T^2 + 39.750T^{-1}$

$\Delta Gf^\circ = 18.436 + 0.428\times10^{-3}T\ln T + 1.709\times10^{-6}T^2 + 19.875T^{-1} - 23.945\times10^{-3}T$

600.65-2000 K: $\Delta Hf^\circ = 18.088 - 2.992\times10^{-3}T + 0.268\times10^{-6}T^2 + 56.350T^{-1}$

$\Delta Gf^\circ = 18.088 + 2.992\times10^{-3}T\ln T - 0.268\times10^{-6}T^2 + 28.175T^{-1} - 38.606\times10^{-3}T$

Source: Data from Chase (27) who estimated some molecular constants.

PbI_2(c,l)

Lead Diiodide

[Formation: $Pb(c,l) + I_2(c,l,g) = PbI_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.540	41.787	41.787	0	-41.920	-41.484	30.408
300	18.550	41.902	41.789	.034	-41.922	-41.482	30.219
386.8	18.808	46.654	42.367	1.658	-42.062	-41.338	23.357
386.8	18.808	46.654	42.367	1.658	-45.771	-41.338	23.357
400	18.847	47.286	42.519	1.907	-45.864	-41.186	22.502
458.4	19.061	49.862	43.296	3.010	-46.272	-40.474	19.297
458.4	19.061	49.862	43.296	3.010	-56.293	-40.474	19.297
500	19.214	51.524	43.912	3.806	-56.148	-39.043	17.066
600	20.008	55.090	45.483	5.764	-55.780	-35.658	12.988
600.65	20.016	55.112	45.494	5.777	-55.777	-35.634	12.965
600.65	20.016	55.112	45.494	5.777	-56.924	-35.634	12.965
683	21.006	57.742	46.815	7.463	-56.577	-32.739	10.476
683	25.950	65.941	46.815	13.063	-50.977	-32.739	10.476
700	25.950	66.579	47.288	13.504	-50.812	-32.287	10.080
800	25.950	70.044	49.920	16.099	-49.842	-29.704	8.115
900	25.950	73.100	52.329	18.694	-48.863	-27.244	6.616
1000	25.950	75.834	54.545	21.289	-47.879	-24.898	5.441
1100	25.950	78.308	56.595	23.884	-46.890	-22.656	4.501
1105	25.950	78.426	56.694	24.014	-46.840	-22.546	4.459

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
600.65 K, melting point of Pb; $\Delta H°$ = 1.147 kcal/mol.
683 K, melting point of PbI_2; $\Delta H°$ = 5.600 kcal/mol.
1105 K, calculated boiling point to PbI_2(g); $\Delta H°$ = 28.34 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-683 K: $Cp° = 14.946 + 7.982\times10^{-3}T + 1.079\times10^{5}T^{-2}$

$H°- H°_{298} = 14.946\times10^{-3}T + 3.991\times10^{-6}T^2 - 1.079\times10^{2}T^{-1} - 4.449$

683-1105 K: $Cp° = 25.901 + 0.040\times10^{-3}T + 0.101\times10^{5}T^{-2}$

$H°- H°_{298} = 25.901\times10^{-3}T + 0.020\times10^{-6}T^2 - 0.101\times10^{2}T^{-1} - 4.622$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -40.933 - 2.782\times10^{-3}T + 0.735\times10^{-6}T^2 - 66.500T^{-1}$

$\Delta Gf° = -40.933 + 2.782\times10^{-3}T\ln T - 0.735\times10^{-6}T^2 - 33.250T^{-1} - 17.107\times10^{-3}T$

386.8-458.4 K: $\Delta Hf° = -42.388 - 9.186\times10^{-3}T + 2.227\times10^{-6}T^2 - 66.500T^{-1}$

$\Delta Gf° = -42.388 + 9.186\times10^{-3}T\ln T - 2.227\times10^{-6}T^2 - 33.250T^{-1} - 50.923\times10^{-3}T$

458.4-600.65 K: $\Delta Hf° = -57.101 + 1.154\times10^{-3}T + 2.159\times10^{-6}T^2 - 81.800T^{-1}$

$\Delta Gf° = -57.101 - 1.154\times10^{-3}T\ln T - 2.159\times10^{-6}T^2 - 40.900T^{-1} + 44.540\times10^{-3}T$

600.65-683 K: $\Delta Hf° = -57.449 - 1.410\times10^{-3}T + 4.136\times10^{-6}T^2 - 65.200T^{-1}$

$\Delta Gf° = -57.449 + 1.410\times10^{-3}T\ln T - 4.136\times10^{-6}T^2 - 32.600T^{-1} + 29.879\times10^{-3}T$

683-1105 K: $\Delta Hf° = -57.622 + 9.545\times10^{-3}T + 0.165\times10^{-6}T^2 + 32.600T^{-1}$

$\Delta Gf° = -57.622 - 9.545\times10^{-3}T\ln T - 0.165\times10^{-6}T^2 + 16.300T^{-1} + 98.813\times10^{-3}T$

Source: Data from Chase (27).

$PbI_2(g)$
Lead Diiodide (ideal gas)
[Formation: $Pb(c,l) + I_2(c,l,g) = PbI_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	13.770	85.908	85.908	0	-0.760	-13.479	9.880
300	13.772	85.993	85.910	.025	-.771	-13.558	9.877
386.8	13.823	89.500	86.337	1.223	-1.337	-17.186	9.710
386.8	13.823	89.500	86.337	1.223	-5.046	-17.186	9.710
400	13.831	89.964	86.449	1.406	-5.205	-17.598	9.615
458.4	13.848	91.851	87.019	2.215	-5.907	-19.357	9.229
458.4	13.848	91.851	87.019	2.215	-15.928	-19.357	9.229
500	13.860	93.054	87.472	2.791	-16.003	-19.663	8.595
600	13.875	95.582	88.619	4.178	-16.206	-20.379	7.423
600.65	13.875	95.597	88.626	4.187	-16.207	-20.382	7.416
600.65	13.875	95.597	88.626	4.187	-17.354	-20.382	7.416
700	13.884	97.722	89.771	5.566	-17.590	-20.865	6.514
800	13.890	99.576	90.883	6.954	-17.827	-21.314	5.823
900	13.894	101.213	91.942	8.344	-18.053	-21.736	5.278
1000	13.897	102.677	92.944	9.733	-18.275	-22.137	4.838
1100	13.900	104.001	93.889	11.123	-18.491	-22.519	4.474
1200	13.901	105.211	94.784	12.513	-18.700	-22.865	4.164
1300	13.903	106.324	95.629	13.903	-18.906	-23.217	3.903
1400	13.904	107.354	96.430	15.294	-19.111	-23.535	3.674
1500	13.904	108.313	97.190	16.684	-19.318	-23.848	3.475
1600	13.905	109.211	97.915	18.074	-19.526	-24.161	3.300
1700	13.906	110.054	98.604	19.465	-19.735	-24.419	3.139
1800	13.906	110.849	99.262	20.856	-19.945	-24.690	2.998
1900	13.907	111.600	99.892	22.246	-20.158	-24.946	2.869
2000	13.907	112.314	100.496	23.637	-20.371	-25.195	2.753

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; $\Delta H° = 3.709$ kcal/mol.
458.4 K, boiling point of I_2; $\Delta H° = 10.021$ kcal/mol.
600.65 K, melting point of Pb; $\Delta H° = 1.147$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.912 - 0.002\times10^{-3}T - 0.126\times10^{5}T^{-2}$

$H°- H°_{298} = 13.912\times10^{-3}T - 0.001\times10^{-6}T^2 + 0.126\times10^{2}T^{-1} - 4.190$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = 0.486 - 3.816\times10^{-3}T - 3.257\times10^{-6}T^2 + 54.000T^{-1}$

$\Delta Gf° = 0.486 + 3.816\times10^{-3}T\ln T + 3.257\times10^{-6}T^2 + 27.000T^{-1} - 69.856\times10^{-3}T$

386.8-458.4 K: $\Delta Hf° = -0.969 - 10.220\times10^{-3}T - 1.765\times10^{-6}T^2 + 54.000T^{-1}$

$\Delta Gf° = -0.969 + 10.220\times10^{-3}T\ln T + 1.765\times10^{-6}T^2 + 27.000T^{-1} - 103.672\times10^{-3}T$

458.4-600.65 K: $\Delta Hf° = -15.682 + 0.120\times10^{-3}T - 1.833\times10^{-6}T^2 + 38.700T^{-1}$

$\Delta Gf° = -15.682 - 0.120\times10^{-3}T\ln T + 1.833\times10^{-6}T^2 + 19.350T^{-1} - 8.209\times10^{-3}T$

600.65-2000 K: $\Delta Hf° = -16.030 - 2.444\times10^{-3}T + 0.144\times10^{-6}T^2 + 55.300T^{-1}$

$\Delta Gf° = -16.030 + 2.444\times10^{-3}T\ln T - 0.144\times10^{-6}T^2 + 27.650T^{-1} - 22.870\times10^{-3}T$

Source: Data from Chase (27) who estimated most molecular constants.

$PbI_4(g)$

Lead Tetraiodide (ideal gas)

[Formation: $Pb(c,l) + 2I_2(c,l,g) = PbI_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	25.409	111.411	111.411	0	-53.649	-65.696	48.156
300	25.414	111.568	111.411	.047	-53.662	-65.770	47.913
386.8	25.571	118.050	112.203	2.261	-54.421	-69.180	39.088
386.8	25.571	118.050	112.203	2.261	-61.839	-69.180	39.088
400	25.595	118.908	112.410	2.599	-62.097	-69.427	37.932
458.4	25.645	122.400	113.466	4.095	-63.236	-70.414	33.571
458.4	25.645	122.400	113.466	4.095	-83.278	-70.414	33.571
500	25.680	124.629	114.303	5.163	-83.234	-69.245	30.267
600	25.726	129.316	116.428	7.733	-83.151	-66.460	24.208
600.65	25.726	129.344	116.442	7.750	-83.150	-66.440	24.174
600.65	25.726	129.344	116.442	7.750	-84.297	-66.440	24.174
700	25.754	133.284	118.558	10.308	-84.247	-63.491	19.822
800	25.773	136.724	120.619	12.884	-84.197	-60.525	16.534
900	25.785	139.761	122.581	15.462	-84.139	-57.570	13.980
1000	25.794	142.478	124.437	18.041	-84.076	-54.624	11.938
1100	25.801	144.937	126.191	20.621	-84.009	-51.690	10.270
1200	25.806	147.182	127.848	23.201	-83.937	-48.743	8.877
1300	25.810	149.248	129.416	25.782	-83.861	-45.826	7.704
1400	25.813	151.160	130.901	28.363	-83.788	-42.897	6.696
1500	25.816	152.941	132.311	30.945	-83.716	-39.983	5.826
1600	25.818	154.608	133.654	33.526	-83.647	-37.087	5.066
1700	25.820	156.173	134.933	36.108	-83.581	-34.154	4.391
1800	25.821	157.649	136.155	38.690	-83.517	-31.250	3.794
1900	25.822	159.045	137.323	41.272	-83.457	-28.347	3.261
2000	25.823	160.369	138.441	43.855	-83.398	-25.448	2.781

*Data estimated.

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
600.65 K, melting point of Pb; $\Delta H°$ = 1.147 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 25.829 + 0.002\times10^{-3}T - 0.374\times10^{5}T^{-2}$

$H°- H°_{298} = 25.829\times10^{-3}T + 0.001\times10^{-6}T^2 + 0.374\times10^{2}T^{-1} - 7.826$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -52.067 - 4.776\times10^{-3}T - 4.747\times10^{-6}T^2 + 78.800T^{-1}$

$\Delta Gf° = -52.067 + 4.776\times10^{-3}T\ln T + 4.747\times10^{-6}T^2 + 39.400T^{-1} - 74.780\times10^{-3}T$

386.8-458.4 K: $\Delta Hf° = -54.978 - 17.584\times10^{-3}T - 1.763\times10^{-6}T^2 + 78.800T^{-1}$

$\Delta Gf° = -54.978 + 17.584\times10^{-3}T\ln T + 1.763\times10^{-6}T^2 + 39.400T^{-1} - 142.411\times10^{-3}T$

458.4-600.65 K: $\Delta Hf° = -84.404 + 3.096\times10^{-3}T - 1.899\times10^{-6}T^2 + 48.200T^{-1}$

$\Delta Gf° = -84.404 - 3.096\times10^{-3}T\ln T + 1.899\times10^{-6}T^2 + 24.100T^{-1} + 48.515\times10^{-3}T$

600.65-2000 K: $\Delta Hf° = -84.752 + 0.532\times10^{-3}T + 0.078\times10^{-6}T^2 + 64.800T^{-1}$

$\Delta Gf° = -84.752 - 0.532\times10^{-3}T\ln T - 0.078\times10^{-6}T^2 + 32.400T^{-1} + 33.854\times10^{-3}T$

Source: Data are estimates from Chase (27).

$PrBr_3(c,l)$

Praseodymium Tribromide

[Formation: $Pr(c,l) + 1.5Br_2(l,g) = PrBr_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	24.300	46.000	46.000	0	-213.000	-205.177	150.397
300	24.300	46.150	46.000	.045	-213.016	-205.128	149.433
332.6	24.691	48.677	46.141	.844	-213.315	-204.255	134.214
332.6	24.691	48.677	46.141	.844	-223.913	-204.255	134.214
400	25.500	53.313	46.971	2.537	-223.555	-200.310	109.443
500	26.400	59.097	48.835	5.131	-222.978	-194.563	85.042
600	27.200	63.982	50.962	7.812	-222.359	-188.942	68.821
700	28.000	68.232	53.132	10.570	-221.718	-183.422	57.266
800	28.700	72.012	55.260	13.402	-221.053	-177.995	48.625
900	29.400	75.431	57.314	16.305	-220.375	-172.648	41.924
966	29.800	77.527	58.624	18.260	-219.918	-169.166	38.272
966	35.000	89.225	58.624	29.560	-208.618	-169.166	38.272
1000	35.000	90.436	59.686	30.750	-208.212	-167.785	36.669
1068	35.000	92.738	61.717	33.130	-207.421	-165.068	33.778
1068	35.000	92.738	61.717	33.130	-208.178	-165.068	33.778
1100	35.000	93.771	62.635	34.250	-207.785	-163.783	32.540
1200	35.000	96.817	65.359	37.750	-206.559	-159.836	29.110
1204	35.000	96.933	65.463	37.890	-206.510	-159.674	28.984
1204	35.000	96.933	65.463	37.890	-208.156	-159.674	28.984
1300	35.000	99.618	67.887	41.250	-207.085	-155.852	26.201

*Data estimated except enthalpy of formation at 298 K and temperature and enthalpy of fusion.

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
966 K, melting point of $PrBr_3$; $\Delta H°$ = 11.300 kcal/mol.
1068 K, α - β transition point of Pr; $\Delta H°$ = 0.757 kcal/mol.
1204 K, melting point of Pr; $\Delta H°$ = 1.646 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-966 K: $Cp° = 23.330 + 6.874\times10^{-3}T - 0.958\times10^{5}T^{-2}$

$H°- H°_{298} = 23.330\times10^{-3}T + 3.437\times10^{-6}T^2 + 0.958\times10^{2}T^{-1} - 7.583$

966-1300 K: $Cp° = 35.000$

$H°- H°_{298} = 35.000\times10^{-3}T - 4.250$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -211.264 - 7.976\times10^{-3}T + 0.924\times10^{-6}T^2 + 167.100T^{-1}$

$\Delta Gf° = -211.264 + 7.976\times10^{-3}T\ln T - 0.924\times10^{-6}T^2 + 83.550T^{-1} - 25.694\times10^{-3}T$

332.6-966 K: $\Delta Hf° = -226.265 + 5.765\times10^{-3}T + 0.691\times10^{-6}T^2 + 120.000T^{-1}$

$\Delta Gf° = -226.265 - 5.765\times10^{-3}T\ln T - 0.691\times10^{-6}T^2 + 60.000T^{-1} + 99.339\times10^{-3}T$

966-1068 K: $\Delta Hf° = -222.932 + 17.435\times10^{-3}T - 2.746\times10^{-6}T^2 + 24.200T^{-1}$

$\Delta Gf° = -222.932 - 17.435\times10^{-3}T\ln T + 2.746\times10^{-6}T^2 + 12.100T^{-1} + 172.829\times10^{-3}T$

1068-1204 K: $\Delta Hf° = -221.298 + 12.415\times10^{-3}T - 0.083\times10^{-6}T^2 - 47.100T^{-1}$

$\Delta Gf° = -221.298 - 12.415\times10^{-3}T\ln T + 0.083\times10^{-6}T^2 - 23.550T^{-1} + 139.168\times10^{-3}T$

1204-1300 K: $\Delta Hf° = -221.644 + 11.335\times10^{-3}T - 0.083\times10^{-6}T^2 - 47.100T^{-1}$

$\Delta Gf° = -221.644 - 11.335\times10^{-3}T\ln T + 0.083\times10^{-6}T^2 - 23.550T^{-1} + 131.794\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Hurtgen (103). Entropy at 298 K estimated. High-temperature data derived from estimated heat capacities based on Dworkin (68). Temperature and enthalpy of fusion from Dworkin (68).

$PrBr_3(g)$

Praseodymium Tribromide (ideal gas)

[Formation: $Pr(c,l) + 1.5Br_2(l,g) = PrBr_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.132	95.852	95.852	0	-142.100	-149.140	109.321
300	19.141	95.971	95.854	.035	-142.126	-149.184	108.679
332.6	19.259	97.952	95.965	.661	-142.598	-149.927	98.515
332.6	19.259	97.952	95.965	.661	-153.195	-149.927	98.515
400	19.502	101.531	96.608	1.969	-153.223	-149.265	81.553
500	19.774	105.912	98.046	3.933	-153.276	-148.269	64.807
600	20.037	109.541	99.668	5.924	-153.347	-147.266	53.641
700	20.297	112.649	101.306	7.940	-153.448	-146.244	45.659
800	20.544	115.376	102.897	9.983	-153.572	-145.205	39.668
900	20.769	117.808	104.421	12.048	-153.732	-144.144	35.003
1000	20.968	120.007	105.872	14.135	-153.927	-143.071	31.268
1068	21.084	121.391	106.816	15.565	-154.085	-142.334	29.126
1068	21.084	121.391	106.816	15.565	-154.842	-142.334	29.126
1100	21.138	122.014	107.249	16.241	-154.894	-141.959	28.204
1200	21.278	123.859	108.557	18.362	-155.047	-140.775	25.638
1204	21.282	123.930	108.608	18.447	-155.053	-140.720	25.543
1204	21.282	123.930	108.608	18.447	-156.699	-140.720	25.543
1300	21.388	125.567	109.801	20.496	-156.939	-139.440	23.442
1400	21.471	127.155	110.984	22.639	-157.182	-138.085	21.556
1500	21.528	128.639	112.113	24.789	-157.421	-136.712	19.919
1600	21.562	130.029	113.189	26.944	-157.658	-135.327	18.485
1700	21.577	131.337	114.219	29.101	-157.893	-133.914	17.216
1800	21.575	132.570	115.204	31.258	-158.129	-132.509	16.089
1900	21.560	133.736	116.149	33.415	-158.367	-131.067	15.076
2000	21.534	134.842	117.057	35.570	-158.610	-129.621	14.164

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.
1068 K, α - β transition point of Pr; $\Delta H° = 0.757$ kcal/mol.
1204 K, melting point of Pr; $\Delta H° = 1.646$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.590 + 1.276\times10^{-3}T - 0.745\times10^{5}T^{-2}$

$H°- H°_{298} = 19.590\times10^{-3}T + 0.638\times10^{-6}T^2 + 0.745\times10^{2}T^{-1} - 6.147$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -138.929 - 11.716\times10^{-3}T - 1.875\times10^{-6}T^2 + 145.800T^{-1}$

$\Delta Gf° = -138.929 + 11.716\times10^{-3}T\ln T + 1.875\times10^{-6}T^2 + 72.900T^{-1} - 102.384\times10^{-3}T$

332.6-1068 K: $\Delta Hf° = -153.930 + 2.025\times10^{-3}T - 2.108\times10^{-6}T^2 + 98.700T^{-1}$

$\Delta Gf° = -153.930 - 2.025\times10^{-3}T\ln T + 2.108\times10^{-6}T^2 + 49.350T^{-1} + 22.649\times10^{-3}T$

1068-1204 K: $\Delta Hf° = -152.296 - 2.995\times10^{-3}T + 0.556\times10^{-6}T^2 + 27.400T^{-1}$

$\Delta Gf° = -152.296 + 2.995\times10^{-3}T\ln T - 0.556\times10^{-6}T^2 + 13.700T^{-1} - 11.013\times10^{-3}T$

1204-2000 K: $\Delta Hf° = -152.642 - 4.075\times10^{-3}T + 0.556\times10^{-6}T^2 + 27.400T^{-1}$

$\Delta Gf° = -152.642 + 4.075\times10^{-3}T\ln T - 0.556\times10^{-6}T^2 + 13.700T^{-1} - 18.387\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

$PrCl_3(c,l)$
Praseodymium Trichloride
[Formation: $Pr(c,l) + 1.5Cl_2(g) = PrCl_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	23.650	36.640	36.640	0	-252.600	-234.423	171.835
300*	23.700	36.790	36.643	.044	-252.590	-234.311	170.694
400	25.200	43.810	37.590	2.488	-252.059	-228.296	124.733
500	26.500	49.570	39.428	5.071	-251.449	-222.422	97.219
600	27.600	54.490	41.533	7.774	-250.780	-216.682	78.925
700	28.600	58.820	43.697	10.586	-250.063	-211.052	65.893
800	29.600	62.710	45.838	13.498	-249.304	-205.534	56.149
900	30.600	66.250	47.909	16.507	-248.507	-200.100	48.590
1000	31.600	69.530	49.914	19.616	-247.671	-194.773	42.567
1059	32.300	71.360	51.060	21.500	-247.159	-191.676	39.556
1059	32.000	82.790	51.060	33.600	-235.059	-191.676	39.556
1068	32.000	83.061	51.330	33.888	-234.982	-191.310	39.148
1068	32.000	83.061	51.330	33.888	-235.739	-191.310	39.148
1100	32.000	84.000	52.262	34.912	-235.440	-189.978	37.745
1200	32.000	86.780	55.020	38.112	-234.509	-185.880	33.853
1204	32.000	86.886	55.126	38.240	-234.472	-185.712	33.710
1204	32.000	86.886	55.126	38.240	-236.118	-185.712	33.710
1300	32.000	89.350	57.572	41.312	-235.331	-181.736	30.552
1400	32.000	91.720	59.926	44.512	-234.514	-177.643	27.731
1500	32.000	93.950	62.142	47.712	-233.700	-173.641	25.299

*Data 300-1000 K estimated.

Phase changes: 1059 K, melting point of $PrCl_3$; ΔH° = 12.100 kcal/mol.
1068 K, α - β transition point of Pr; ΔH° = 0.757 kcal/mol.
1204 K, melting point of Pr; ΔH° = 1.646 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1059 K: $Cp^\circ = 22.020 + 9.718\times10^{-3}T - 1.127\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 22.020\times10^{-3}T + 4.859\times10^{-6}T^2 + 1.127\times10^{2}T^{-1} - 7.375$

1059-1500 K: $Cp^\circ = 32.000$
$H^\circ - H^\circ_{298} = 32.000\times10^{-3}T - 0.288$

Formation equations (kcal/mol):

298.15-1059 K: $\Delta Hf^\circ = -254.431 + 4.610\times10^{-3}T + 2.064\times10^{-6}T^2 + 81.550T^{-1}$
$\Delta Gf^\circ = -254.431 - 4.610\times10^{-3}T\ln T - 2.064\times10^{-6}T^2 + 40.775T^{-1} + 93.527\times10^{-3}T$

1059-1068 K: $\Delta Hf^\circ = -247.344 + 14.590\times10^{-3}T - 2.795\times10^{-6}T^2 - 31.150T^{-1}$
$\Delta Gf^\circ = -247.344 - 14.590\times10^{-3}T\ln T + 2.795\times10^{-6}T^2 - 15.575T^{-1} + 151.251\times10^{-3}T$

1068-1204 K: $\Delta Hf^\circ = -245.711 + 9.570\times10^{-3}T - 0.132\times10^{-6}T^2 - 102.450T^{-1}$
$\Delta Gf^\circ = -245.711 - 9.570\times10^{-3}T\ln T + 0.132\times10^{-6}T^2 - 51.225T^{-1} + 117.590\times10^{-3}T$

1204-1500 K: $\Delta Hf^\circ = -246.056 + 8.490\times10^{-3}T - 0.132\times10^{-6}T^2 - 102.450T^{-1}$
$\Delta Gf^\circ = -246.056 - 8.490\times10^{-3}T\ln T + 0.132\times10^{-6}T^2 - 51.225T^{-1} + 110.216\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (207). Low-temperature heat capacities and entropy at 298 K from Sommers (219). High-temperature data between 298 K and 1059 K estimated. Values at 1059 K, enthalpy of fusion, and heat capacity of liquid based on Dworkin (66).

$PrCl_3(g)$

Praseodymium Trichloride (ideal gas)

[Formation: $Pr(c,l) + 1.5Cl_2(g) = PrCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.732	89.353	89.353	0	-174.800	-172.340	126.327
300	18.745	89.469	89.353	.035	-174.799	-172.324	125.536
400	19.261	94.939	90.097	1.937	-174.810	-171.498	93.701
500	19.613	99.276	91.512	3.882	-174.838	-170.664	74.596
600	19.924	102.880	93.115	5.859	-174.895	-169.831	61.860
700	20.212	105.973	94.736	7.866	-174.983	-168.979	52.757
800	20.478	108.690	96.315	9.900	-175.102	-168.116	45.927
900	20.717	111.116	97.827	11.960	-175.253	-167.226	40.607
1000	20.926	113.310	99.267	14.043	-175.443	-166.326	36.350
1068	21.046	114.691	100.205	15.471	-175.599	-165.708	33.909
1068	21.046	114.691	100.205	15.471	-176.356	-165.708	33.909
1100	21.103	115.313	100.636	16.145	-176.407	-165.389	32.859
1200	21.249	117.155	101.937	18.262	-176.559	-164.380	29.937
1204	21.254	117.226	101.987	18.347	-176.565	-164.332	29.829
1204	21.254	117.226	101.987	18.347	-178.211	-164.332	29.829
1300	21.363	118.861	103.174	20.393	-178.450	-163.219	27.439
1400	21.449	120.447	104.351	22.534	-178.692	-162.039	25.295
1500	21.509	121.929	105.474	24.682	-178.930	-160.839	23.434
1600	21.545	123.319	106.547	26.835	-179.167	-159.632	21.804
1700	21.562	124.626	107.572	28.991	-179.402	-158.389	20.362
1800	21.562	125.858	108.554	31.147	-179.639	-157.160	19.082
1900	21.548	127.024	109.496	33.303	-179.878	-155.893	17.932
2000	21.523	128.128	110.400	35.456	-180.125	-154.618	16.896

Phase changes: 1068 K, α - β transition point of Pr; $\Delta H°$ = 0.757 kcal/mol.
1204 K, melting point of Pr; $\Delta H°$ = 1.646 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.560 + 1.294\times10^{-3}T - 1.078\times10^{5}T^{-2}$

$H°- H°_{298} = 19.560\times10^{-3}T + 0.647\times10^{-6}T^{2} + 1.078\times10^{2}T^{-1} - 6.251$

Formation equations (kcal/mol):

298.15-1068 K: $\Delta Hf° = -175.507 + 2.149\times10^{-3}T - 2.148\times10^{-6}T^{2} + 76.650T^{-1}$

$\Delta Gf° = -175.507 - 2.149\times10^{-3}T\ln T + 2.148\times10^{-6}T^{2} + 38.325T^{-1} + 21.799\times10^{-3}T$

1068-1204 K: $\Delta Hf° = -173.873 - 2.871\times10^{-3}T + 0.515\times10^{-6}T^{2} + 5.350T^{-1}$

$\Delta Gf° = -173.873 + 2.871\times10^{-3}T\ln T - 0.515\times10^{-6}T^{2} + 2.675T^{-1} - 11.863\times10^{-3}T$

1204-2000 K: $\Delta Hf° = -174.219 - 3.951\times10^{-3}T + 0.515\times10^{-6}T^{2} + 5.350T^{-1}$

$\Delta Gf° = -174.219 + 3.951\times10^{-3}T\ln T - 0.515\times10^{-6}T^{2} + 2.675T^{-1} - 19.237\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Hannay (96). Other data based on Myers (165) and Dieke (56).

PrF_3(c,l)

Praseodymium Trifluoride

[Formation: $Pr(c,l) + 1.5F_2(g) = PrF_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	22.140	28.970	28.970	0	-403.700	-385.404	282.505
300	22.176	29.107	28.970	.041	-403.692	-385.291	280.681
400	23.817	35.726	29.861	2.346	-403.207	-379.226	207.197
500	25.020	41.176	31.596	4.790	-402.664	-373.292	163.164
600	25.917	45.821	33.589	7.339	-402.090	-367.478	133.852
700	26.580	49.868	35.631	9.966	-401.513	-361.753	112.943
800	27.060	53.451	37.640	12.649	-400.947	-356.113	97.284
900	27.406	56.659	39.578	15.373	-400.406	-350.533	85.120
1000	27.663	59.561	41.434	18.127	-399.904	-345.022	75.404
1068	27.806	61.385	42.646	20.013	-399.590	-341.306	69.842
1068	27.806	61.385	42.646	20.013	-400.347	-341.306	69.842
1100	27.873	62.207	43.203	20.904	-400.176	-339.541	67.460
1200	28.080	64.641	44.889	23.702	-399.634	-334.052	60.838
1204	28.090	64.734	44.955	23.814	-399.612	-333.826	60.595
1204	28.090	64.734	44.955	23.814	-401.258	-333.826	60.595
1300	28.325	66.898	46.496	26.522	-400.825	-328.467	55.220
1400	28.652	69.009	48.030	29.370	-400.354	-322.923	50.410
1500	29.102	71.000	49.496	32.256	-399.849	-317.407	46.246
1600	29.717	72.897	50.900	35.196	-399.297	-311.933	42.608
1672	30.285	74.217	51.875	37.355	-398.857	-307.997	40.258
1672	31.250	82.410	51.875	51.055	-385.157	-307.997	40.258
1700	31.250	82.929	52.382	51.930	-384.952	-306.706	39.429
1800	31.250	84.716	54.130	55.055	-384.222	-302.140	36.684

Phase changes: 1068 K, α - β transition point of Pr; $\Delta H°$ = 0.757 kcal/mol.
1204 K, melting point of Pr; $\Delta H°$ = 1.646 kcal/mol.
1672 K, melting point of PrF_3; $\Delta H°$ = 13.700 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1672 K: $Cp° = 24.874 + 3.008\times10^{-3}T - 3.226\times10^{5}T^{-2}$

$H°- H°_{298} = 24.874\times10^{-3}T + 1.504\times10^{-6}T^2 + 3.226\times10^{2}T^{-1} - 8.632$

1672-1800 K: $Cp° = 31.250$

$H°- H°_{298} = 31.250\times10^{-3}T - 1.195$

Formation equations (kcal/mol):

298.15-1068 K: $\Delta Hf° = -406.757 + 7.942\times10^{-3}T - 1.420\times10^{-6}T^2 + 243.150T^{-1}$

$\Delta Gf° = -406.757 - 7.942\times10^{-3}T\ln T + 1.420\times10^{-6}T^2 + 121.575T^{-1} + 115.078\times10^{-3}T$

1068-1204 K: $\Delta Hf° = -405.124 + 2.922\times10^{-3}T + 1.243\times10^{-6}T^2 + 171.850T^{-1}$

$\Delta Gf° = -405.124 - 2.922\times10^{-3}T\ln T - 1.243\times10^{-6}T^2 + 85.925T^{-1} + 81.416\times10^{-3}T$

1204-1672 K: $\Delta Hf° = -405.469 + 1.842\times10^{-3}T + 1.243\times10^{-6}T^2 + 171.850T^{-1}$

$\Delta Gf° = -405.469 - 1.842\times10^{-3}T\ln T - 1.243\times10^{-6}T^2 + 85.925T^{-1} + 74.043\times10^{-3}T$

1672-1800 K: $\Delta Hf° = -398.032 + 8.218\times10^{-3}T - 0.261\times10^{-6}T^2 - 150.750T^{-1}$

$\Delta Gf° = -398.032 - 8.218\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 - 75.375T^{-1} + 114.459\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Johnson (111). Low-temperature heat capacities and entropy at 298 K from Lyon (145). High-temperature data based on Spedding (223).

$PrF_3(g)$

Praseodymium Trifluoride (ideal gas)

[Formation: $Pr(c,l) + 1.5F_2(g) = PrF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	17.303	81.103	81.103	0	-300.700	-297.948	218.399
300	17.327	81.210	81.103	.032	-300.701	-297.931	217.040
400	18.313	86.342	81.797	1.818	-300.736	-297.000	162.271
500	18.955	90.501	83.133	3.684	-300.770	-296.060	129.406
600	19.445	94.002	84.662	5.604	-300.825	-295.121	107.496
700	19.851	97.031	86.217	7.570	-300.909	-294.163	91.841
800	20.196	99.705	87.739	9.573	-301.023	-293.192	80.095
900	20.491	102.101	89.204	11.607	-301.172	-292.197	70.954
1000	20.741	104.273	90.604	13.669	-301.362	-291.192	63.639
1068	20.883	105.642	91.518	15.085	-301.518	-290.502	59.446
1068	20.883	105.642	91.518	15.085	-302.275	-290.502	59.446
1100	20.950	106.260	91.938	15.754	-302.326	-290.149	57.647
1200	21.119	108.091	93.209	17.858	-302.478	-289.036	52.640
1204	21.124	108.161	93.259	17.942	-302.484	-288.984	52.456
1204	21.124	108.161	93.259	17.942	-304.130	-288.984	52.456
1300	21.252	109.787	94.420	19.977	-304.370	-287.768	48.378
1400	21.353	111.365	95.574	22.107	-304.617	-286.484	44.722
1500	21.425	112.841	96.677	24.246	-304.859	-285.179	41.550
1600	21.472	114.226	97.732	26.391	-305.102	-283.865	38.774
1700	21.497	115.528	98.740	28.540	-305.341	-282.515	36.319
1800	21.503	116.757	99.707	30.690	-305.587	-281.179	34.139
1900	21.495	117.920	100.636	32.840	-305.833	-279.807	32.185
2000	21.476	119.022	101.528	34.989	-306.087	-278.424	30.424

Phase changes: 1068 K, α - β transition point of Pr; $\Delta H° = 0.757$ kcal/mol.
1204 K, melting point of Pr; $\Delta H° = 1.646$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.293 + 1.444\times10^{-3}T - 2.152\times10^{5}T^{-2}$

$H°-H°_{298} = 19.293\times10^{-3}T + 0.722\times10^{-6}T^2 + 2.152\times10^{2}T^{-1} - 6.538$

Formation equations (kcal/mol):

298.15-1068 K: $\Delta Hf° = -301.664 + 2.361\times10^{-3}T - 2.202\times10^{-6}T^2 + 135.750T^{-1}$

$\Delta Gf° = -301.664 - 2.361\times10^{-3}T\ln T + 2.202\times10^{-6}T^2 + 67.875T^{-1} + 24.495\times10^{-3}T$

1068-1204 K: $\Delta Hf° = -300.030 - 2.659\times10^{-3}T + 0.461\times10^{-6}T^2 + 64.450T^{-1}$

$\Delta Gf° = -300.030 + 2.659\times10^{-3}T\ln T - 0.461\times10^{-6}T^2 + 32.225T^{-1} - 9.166\times10^{-3}T$

1204-2000 K: $\Delta Hf° = -300.376 - 3.739\times10^{-3}T + 0.461\times10^{-6}T^2 + 64.450T^{-1}$

$\Delta Gf° = -300.376 + 3.739\times10^{-3}T\ln T - 0.461\times10^{-6}T^2 + 32.225T^{-1} - 16.540\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

$PrI_3(c,l)$

Praseodymium Triiodide

[Formation: $Pr(c,l) + 1.5I_2(c,l,g) = PrI_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	23.800	54.700	54.700	0	-156.400	-155.026	113.636
300	23.900	54.848	54.701	.044	-156.404	-155.018	112.929
386.8	25.028	61.071	55.455	2.172	-156.665	-154.584	87.342
386.8	25.028	61.071	55.455	2.172	-162.229	-154.584	87.342
400	25.200	61.914	55.654	2.504	-162.369	-154.321	84.316
458.4	25.784	65.396	56.677	3.997	-162.965	-153.100	72.992
458.4	25.784	65.396	56.677	3.997	-177.997	-153.100	72.992
500	26.200	67.654	57.498	5.078	-177.766	-150.848	65.935
600	27.100	72.511	59.606	7.743	-177.176	-145.527	53.007
700	27.800	76.742	61.758	10.489	-176.557	-140.299	43.803
800	28.600	80.508	63.871	13.310	-175.911	-135.162	36.924
900	29.300	83.916	65.912	16.204	-175.251	-130.102	31.593
1000	30.000	87.040	67.870	19.170	-174.574	-125.121	27.345
1011	30.100	87.368	68.080	19.500	-174.500	-124.578	26.930
1011	34.000	99.930	68.080	32.200	-161.800	-124.578	26.930
1068	34.000	101.795	69.831	34.138	-161.200	-122.504	25.068
1068	34.000	101.795	69.831	34.138	-161.957	-122.504	25.068
1100	34.000	102.799	70.775	35.226	-161.598	-121.328	24.105
1200	34.000	105.757	73.569	38.626	-160.481	-117.715	21.439
1204	34.000	105.870	73.676	38.762	-160.437	-117.566	21.340
1204	34.000	105.870	73.676	38.762	-162.083	-117.566	21.340
1300	34.000	108.479	76.151	42.026	-161.113	-114.056	19.174

*Data estimated except enthalpy of formation at 298 K and temperature and enthalpy of fusion.

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
1011 K, melting point of PrI_3; $\Delta H°$ = 12.700 kcal/mol.
1068 K, α - β transition point of Pr; $\Delta H°$ = 0.757 kcal/mol.
1204 K, melting point of Pr; $\Delta H°$ = 1.646 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1011 K: $Cp° = 23.520 + 6.622\times10^{-3}T - 1.506\times10^{5}T^{-2}$

$H°- H°_{298} = 23.520\times10^{-3}T + 3.311\times10^{-6}T^{2} + 1.506\times10^{2}T^{-1} - 7.812$

1011-1300 K: $Cp° = 34.000$

$H°- H°_{298} = 34.000\times10^{-3}T - 2.174$

PrI_3(c,l) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -157.013 + 0.034\times10^{-3}T - 1.590\times10^{-6}T^2 + 221.900T^{-1}$

$\Delta Gf^\circ = -157.013 - 0.034\times10^{-3}T\ln T + 1.590\times10^{-6}T^2 + 110.950T^{-1} + 5.138\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -159.196 - 9.571\times10^{-3}T + 0.648\times10^{-6}T^2 + 221.900T^{-1}$

$\Delta Gf^\circ = -159.196 + 9.571\times10^{-3}T\ln T - 0.648\times10^{-6}T^2 + 110.950T^{-1} - 45.585\times10^{-3}T$

458.4-1011 K: $\Delta Hf^\circ = -181.266 + 5.939\times10^{-3}T + 0.546\times10^{-6}T^2 + 198.950T^{-1}$

$\Delta Gf^\circ = -181.266 - 5.939\times10^{-3}T\ln T - 0.546\times10^{-6}T^2 + 99.475T^{-1} + 97.609\times10^{-3}T$

1011-1068 K: $\Delta Hf^\circ = -175.628 + 16.419\times10^{-3}T - 2.765\times10^{-6}T^2 + 48.350T^{-1}$

$\Delta Gf^\circ = -175.628 - 16.419\times10^{-3}T\ln T + 2.765\times10^{-6}T^2 + 24.175T^{-1} + 161.267\times10^{-3}T$

1068-1204 K: $\Delta Hf^\circ = -173.994 + 11.399\times10^{-3}T - 0.102\times10^{-6}T^2 - 22.950T^{-1}$

$\Delta Gf^\circ = -173.994 - 11.399\times10^{-3}T\ln T + 0.102\times10^{-6}T^2 - 11.475T^{-1} + 127.606\times10^{-3}T$

1204-1300 K: $\Delta Hf^\circ = -174.340 + 10.319\times10^{-3}T - 0.102\times10^{-6}T^2 - 22.950T^{-1}$

$\Delta Gf^\circ = -174.340 - 10.319\times10^{-3}T\ln T + 0.102\times10^{-6}T^2 - 11.475T^{-1} + 120.232\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (207). Entropy at 298 K estimated. High-temperature data derived from estimated heat capacities based on Dworkin (66). Temperature and enthalpy of fusion from Dworkin (66).

$PrI_3(g)$

Praseodymium Triiodide (ideal gas)

[Formation: $Pr(c,l) + 1.5I_2(c,l,g) = PrI_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.494	102.791	102.791	0	-90.600	-103.565	75.914
300	19.499	102.912	102.792	.036	-90.612	-103.645	75.504
386.8	19.685	107.891	103.400	1.737	-91.301	-107.330	60.643
386.8	19.685	107.891	103.400	1.737	-96.864	-107.330	60.643
400	19.713	108.552	103.560	1.997	-97.076	-107.684	58.835
458.4	19.829	111.246	104.371	3.151	-98.010	-109.163	52.045
458.4	19.829	111.246	104.371	3.151	-113.042	-109.163	52.045
500	19.912	112.972	105.016	3.978	-113.066	-108.807	47.559
600	20.134	116.622	106.655	5.980	-113.139	-107.956	39.323
700	20.369	119.743	108.306	8.006	-113.240	-107.082	33.432
800	20.599	122.478	109.910	10.054	-113.368	-106.194	29.010
900	20.813	124.917	111.445	12.125	-113.530	-105.281	25.565
1000	21.003	127.120	112.904	14.216	-113.728	-104.355	22.807
1068	21.115	128.505	113.853	15.648	-113.889	-103.719	21.224
1068	21.115	128.505	113.853	15.648	-114.646	-103.719	21.224
1100	21.167	129.129	114.288	16.325	-114.700	-103.392	20.542
1200	21.303	130.977	115.604	18.448	-114.859	-102.357	18.642
1204	21.307	131.048	115.655	18.533	-114.865	-102.309	18.571
1204	21.307	131.048	115.655	18.533	-116.511	-102.309	18.571
1300	21.410	132.687	116.853	20.584	-116.756	-101.168	17.008
1400	21.489	134.276	118.041	22.729	-117.006	-99.960	15.604
1500	21.544	135.761	119.174	24.881	-117.250	-98.735	14.385
1600	21.576	137.153	120.255	27.037	-117.493	-97.496	13.317
1700	21.589	138.461	121.287	29.196	-117.735	-96.226	12.371
1800	21.586	139.695	122.276	31.355	-117.979	-94.966	11.530
1900	21.570	140.862	123.224	33.512	-118.227	-93.673	10.775
2000	21.543	141.968	124.134	35.668	-118.478	-92.368	10.093

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
1068 K, α - β transition point of Pr; $\Delta H°$ = 0.757 kcal/mol.
1204 K, melting point of Pr; $\Delta H°$ = 1.646 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.609 + 1.264\times10^{-3}T - 0.437\times10^{5}T^{-2}$

$H°- H°_{298} = 19.609\times10^{-3}T + 0.632\times10^{-6}T^{2} + 0.437\times10^{2}T^{-1} - 6.049$

$PrI_3(g)$ - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -89.450 - 3.877\times10^{-3}T - 4.269\times10^{-6}T^2 + 115.000T^{-1}$

$\Delta Gf^\circ = -89.450 + 3.877\times10^{-3}T\ln T + 4.269\times10^{-6}T^2 + 57.500T^{-1} - 71.346\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -91.633 - 13.483\times10^{-3}T - 2.031\times10^{-6}T^2 + 115.000T^{-1}$

$\Delta Gf^\circ = -91.633 + 13.483\times10^{-3}T\ln T + 2.031\times10^{-6}T^2 + 57.500T^{-1} - 122.069\times10^{-3}T$

458.4-1068 K: $\Delta Hf^\circ = -113.703 + 2.027\times10^{-3}T - 2.133\times10^{-6}T^2 + 92.050T^{-1}$

$\Delta Gf^\circ = -113.703 - 2.027\times10^{-3}T\ln T + 2.133\times10^{-6}T^2 + 46.025T^{-1} + 21.125\times10^{-3}T$

1068-1204 K: $\Delta Hf^\circ = -112.069 - 2.993\times10^{-3}T + 0.530\times10^{-6}T^2 + 20.750T^{-1}$

$\Delta Gf^\circ = -112.069 + 2.993\times10^{-3}T\ln T - 0.530\times10^{-6}T^2 + 10.375T^{-1} - 12.536\times10^{-3}T$

1204-2000 K: $\Delta Hf^\circ = -112.415 - 4.073\times10^{-3}T + 0.530\times10^{-6}T^2 + 20.750T^{-1}$

$\Delta Gf^\circ = -112.415 + 4.073\times10^{-3}T\ln T - 0.530\times10^{-6}T^2 + 10.375T^{-1} - 19.910\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

$PuBr_3(c,l)$
Plutonium Tribromide
[Formation: $Pu(c,l) + 1.5Br_2(l,g) = PuBr_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	25.780	46.100	46.100	0	-189.600	-183.074	134.195
300	25.790	46.259	46.100	.048	-189.617	-183.033	133.337
332.6	25.953	48.928	46.248	.891	-189.919	-182.302	119.788
332.6	25.953	48.928	46.248	.891	-200.517	-182.302	119.788
395	26.265	53.416	47.035	2.521	-200.247	-178.913	98.990
395	26.265	53.416	47.035	2.521	-201.067	-178.913	98.990
400	26.290	53.747	47.117	2.652	-201.043	-178.634	97.600
480	26.690	58.575	48.635	4.771	-200.647	-174.189	79.309
480	26.690	58.575	48.635	4.771	-200.782	-174.189	79.309
500	26.790	59.667	49.055	5.306	-200.683	-173.084	75.654
588	27.230	64.045	50.979	7.683	-200.255	-168.262	62.539
588	27.230	64.045	50.979	7.683	-200.395	-168.262	62.539
600	27.290	64.596	51.246	8.010	-200.335	-167.606	61.050
700	27.790	68.840	53.463	10.764	-199.808	-162.192	50.638
730	27.943	70.009	54.119	11.600	-199.641	-160.583	48.075
730	27.943	70.009	54.119	11.600	-199.661	-160.583	48.075
752	28.055	70.840	54.597	12.215	-199.527	-159.407	46.327
752	28.055	70.840	54.597	12.215	-199.967	-159.407	46.327
800	28.300	72.584	55.624	13.568	-199.656	-156.828	42.843
900	28.800	75.947	57.700	16.422	-198.973	-151.519	36.793
913	28.865	76.360	57.963	16.797	-198.881	-150.834	36.106
913	28.865	76.360	57.963	16.797	-199.556	-150.834	36.106
954	29.070	77.632	58.781	17.984	-199.336	-148.651	34.054
954	33.000	91.678	58.781	31.384	-185.936	-148.651	34.054
1000	33.000	93.233	60.331	32.902	-185.503	-146.863	32.096
1100	33.000	96.378	63.467	36.202	-184.566	-143.044	28.420
1200	33.000	99.249	66.331	39.502	-183.631	-139.310	25.371
1300	33.000	101.891	68.966	42.802	-182.698	-135.656	22.806
1400	33.000	104.336	71.406	46.102	-181.767	-132.070	20.617
1500	33.000	106.613	73.678	49.402	-180.839	-128.554	18.730

*Data estimated except enthalpy of formation at 298 K and temperature and enthalpy of fusion.

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
395 K, α - β transition point of Pu; $\Delta H°$ = 0.820 kcal/mol.
480 K, β - γ transition point of Pu; $\Delta H°$ = 0.135 kcal/mol.
588 K, γ - δ transition point of Pu; $\Delta H°$ = 0.140 kcal/mol.
730 K, δ - δ' transition point of Pu; $\Delta H°$ = 0.020 kcal/mol.
752 K, δ' - ε transition point of Pu; $\Delta H°$ = 0.440 kcal/mol.
913 K, melting point of Pu; $\Delta H°$ = 0.675 kcal/mol.
954 K, melting point of $PuBr_3$; $\Delta H°$ = 13.400 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-954 K: $Cp° = 24.290 + 5.000\times10^{-3}T$

$H°- H°_{298} = 24.290\times10^{-3}T + 2.500\times10^{-6}T^2 - 7.464$

954-1500 K: $Cp° = 33.000$

$H°- H°_{298} = 33.000\times10^{-3}T - 0.098$

$PuBr_3$(c,1) - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -187.222 - 6.836\times10^{-3}T - 3.824\times10^{-6}T^2$

$\Delta Gf^\circ = -187.222 + 6.836\times10^{-3}T\ln T + 3.824\times10^{-6}T^2 - 26.180\times10^{-3}T$

332.6-395 K: $\Delta Hf^\circ = -202.222 + 6.905\times10^{-3}T - 4.056\times10^{-6}T^2 - 47.100T^{-1}$

$\Delta Gf^\circ = -202.222 - 6.905\times10^{-3}T\ln T + 4.056\times10^{-6}T^2 - 23.550T^{-1} + 98.853\times10^{-3}T$

395-480 K: $\Delta Hf^\circ = -202.833 + 4.838\times10^{-3}T - 0.167\times10^{-6}T^2 - 47.100T^{-1}$

$\Delta Gf^\circ = -202.833 - 4.838\times10^{-3}T\ln T + 0.167\times10^{-6}T^2 - 23.550T^{-1} + 89.576\times10^{-3}T$

480-588 K: $\Delta Hf^\circ = -203.229 + 5.793\times10^{-3}T - 1.025\times10^{-6}T^2 - 47.100T^{-1}$

$\Delta Gf^\circ = -203.229 - 5.793\times10^{-3}T\ln T + 1.025\times10^{-6}T^2 - 23.550T^{-1} + 95.885\times10^{-3}T$

588-730 K: $\Delta Hf^\circ = -202.339 + 2.018\times10^{-3}T + 2.417\times10^{-6}T^2 - 47.100T^{-1}$

$\Delta Gf^\circ = -202.339 - 2.018\times10^{-3}T\ln T - 2.417\times10^{-6}T^2 - 23.550T^{-1} + 72.324\times10^{-3}T$

730-752 K: $\Delta Hf^\circ = -202.634 + 2.395\times10^{-3}T + 2.417\times10^{-6}T^2 - 47.100T^{-1}$

$\Delta Gf^\circ = -202.634 - 2.395\times10^{-3}T\ln T - 2.417\times10^{-6}T^2 - 23.550T^{-1} + 75.214\times10^{-3}T$

752-913 K: $\Delta Hf^\circ = -203.276 + 2.663\times10^{-3}T + 2.417\times10^{-6}T^2 - 47.100T^{-1}$

$\Delta Gf^\circ = -203.276 - 2.663\times10^{-3}T\ln T - 2.417\times10^{-6}T^2 - 23.550T^{-1} + 77.842\times10^{-3}T$

913-954 K: $\Delta Hf^\circ = -202.245 + 0.795\times10^{-3}T + 2.417\times10^{-6}T^2 - 47.100T^{-1}$

$\Delta Gf^\circ = -202.245 - 0.795\times10^{-3}T\ln T - 2.417\times10^{-6}T^2 - 23.550T^{-1} + 63.979\times10^{-3}T$

954-1500 K: $\Delta Hf^\circ = -194.879 + 9.505\times10^{-3}T - 0.083\times10^{-6}T^2 - 47.100T^{-1}$

$\Delta Gf^\circ = -194.879 - 9.505\times10^{-3}T\ln T + 0.083\times10^{-6}T^2 - 23.550T^{-1} + 113.630\times10^{-3}T$

Sources: Enthalpy of formation from Brown (19). Other data from Oetting (174) who estimated all except temperature and enthalpy of fusion.

$PuCl_3(c,l)$

Plutonium Trichloride

[Formation: $Pu(c,l) + 1.5Cl_2(g) = PuCl_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	24.580	38.000	38.000	0	-229.800	-213.296	156.348
300	24.600	38.152	38.002	.045	-229.793	-213.194	155.310
395	25.170	44.994	38.895	2.409	-229.416	-207.995	115.080
395	25.170	44.994	38.895	2.409	-230.236	-207.995	115.080
400	25.200	45.311	38.973	2.535	-230.214	-207.714	113.488
480	25.680	49.948	40.427	4.570	-229.867	-203.246	92.539
480	25.680	49.948	40.427	4.570	-230.002	-203.246	92.539
500	25.800	50.999	40.829	5.085	-229.915	-202.133	88.351
588	26.328	55.223	42.675	7.379	-229.546	-197.275	73.323
588	26.328	55.223	42.675	7.379	-229.686	-197.275	73.323
600	26.400	55.756	42.931	7.695	-229.632	-196.614	71.616
700	27.000	59.869	45.062	10.365	-229.167	-191.146	59.678
730	27.210	61.006	45.694	11.178	-229.018	-189.519	56.738
730	27.210	61.006	45.694	11.178	-229.038	-189.519	56.738
752	27.364	61.817	46.155	11.778	-228.918	-188.332	54.733
752	27.364	61.817	46.155	11.778	-229.358	-188.332	54.733
800	27.700	63.521	47.146	13.100	-229.070	-185.722	50.736
900	28.300	66.818	49.151	15.900	-228.429	-180.341	43.792
913	28.391	67.225	49.406	16.268	-228.341	-179.647	43.003
913	28.391	67.225	49.406	16.268	-229.016	-179.647	43.003
1000	29.000	69.841	51.071	18.770	-228.559	-174.963	38.238
1033	29.230	70.786	51.685	19.731	-228.375	-173.197	36.642
1033	32.000	85.500	51.685	34.931	-213.175	-173.197	36.642
1100	32.000	87.510	53.805	37.075	-212.610	-170.621	33.899
1200	32.000	90.294	56.731	40.275	-211.770	-166.841	30.385
1300	32.000	92.855	59.413	43.475	-210.933	-163.131	27.424
1400	32.000	95.227	61.888	46.675	-210.099	-159.485	24.896
1500	32.000	97.434	64.184	49.875	-209.268	-155.897	22.714

*Data estimated except enthalpy of formation at 298 K and temperature and enthalpy of fusion.

Phase changes: 395 K, α - β transition point of Pu; ΔH° = 0.820 kcal/mol.
480 K, β - γ transition point of Pu; ΔH° = 0.135 kcal/mol.
588 K, γ - δ transition point of Pu; ΔH° = 0.140 kcal/mol.
730 K, δ - δ' transition point of Pu; ΔH° = 0.020 kcal/mol.
752 K, δ' - ε transition point of Pu; ΔH° = 0.440 kcal/mol.
913 K, melting point of Pu; ΔH° = 0.675 kcal/mol.
1033 K, melting point of $PuCl_3$; ΔH° = 15.200 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1033 K: $Cp^\circ = 22.496 + 6.476\times10^{-3}T + 0.136\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 22.496\times10^{-3}T + 3.238\times10^{-6}T^2 - 0.136\times10^{2}T^{-1} - 6.949$

1033-1500 K: $Cp^\circ = 32.000$

$H^\circ - H^\circ_{298} = 32.000\times10^{-3}T + 1.875$

$PuCl_3$(c,1) - Continued

Formation equations (kcal/mol):

298.15-395 K: $\Delta Hf^\circ = -230.681 + 5.266\times10^{-3}T - 3.368\times10^{-6}T^2 - 116.050T^{-1}$

$\Delta Gf^\circ = -230.681 - 5.266\times10^{-3}T\ln T + 3.368\times10^{-6}T^2 - 58.025T^{-1} + 87.960\times10^{-3}T$

395-480 K: $\Delta Hf^\circ = -231.292 + 3.199\times10^{-3}T + 0.522\times10^{-6}T^2 - 116.050T^{-1}$

$\Delta Gf^\circ = -231.292 - 3.199\times10^{-3}T\ln T - 0.522\times10^{-6}T^2 - 58.025T^{-1} + 78.684\times10^{-3}T$

480-588 K: $\Delta Hf^\circ = -231.688 + 4.153\times10^{-3}T - 0.336\times10^{-6}T^2 - 116.050T^{-1}$

$\Delta Gf^\circ = -231.688 - 4.153\times10^{-3}T\ln T + 0.336\times10^{-6}T^2 - 58.025T^{-1} + 84.992\times10^{-3}T$

588-730 K: $\Delta Hf^\circ = -230.798 + 0.379\times10^{-3}T + 3.106\times10^{-6}T^2 - 116.050T^{-1}$

$\Delta Gf^\circ = -230.798 - 0.379\times10^{-3}T\ln T - 3.106\times10^{-6}T^2 - 58.025T^{-1} + 61.431\times10^{-3}T$

730-752 K: $\Delta Hf^\circ = -231.093 + 0.756\times10^{-3}T + 3.106\times10^{-6}T^2 - 116.050T^{-1}$

$\Delta Gf^\circ = -231.093 - 0.756\times10^{-3}T\ln T - 3.106\times10^{-6}T^2 - 58.025T^{-1} + 64.321\times10^{-3}T$

752-913 K: $\Delta Hf^\circ = -231.735 + 1.023\times10^{-3}T + 3.106\times10^{-6}T^2 - 116.050T^{-1}$

$\Delta Gf^\circ = -231.735 - 1.023\times10^{-3}T\ln T - 3.106\times10^{-6}T^2 - 58.025T^{-1} + 66.949\times10^{-3}T$

913-1033 K: $\Delta Hf^\circ = -230.704 - 0.845\times10^{-3}T + 3.106\times10^{-6}T^2 - 116.050T^{-1}$

$\Delta Gf^\circ = -230.704 + 0.845\times10^{-3}T\ln T - 3.106\times10^{-6}T^2 - 58.025T^{-1} + 53.087\times10^{-3}T$

1033-1500 K: $\Delta Hf^\circ = -221.880 + 8.660\times10^{-3}T - 0.132\times10^{-6}T^2 - 102.450T^{-1}$

$\Delta Gf^\circ = -221.880 - 8.660\times10^{-3}T\ln T + 0.132\times10^{-6}T^2 - 51.225T^{-1} + 107.153\times10^{-3}T$

Source: Data from Oetting (174) who estimated all except enthalpy of formation at 298 K and temperature and enthalpy of fusion.

$PuF_3(c,l)$

Plutonium Trifluoride

[Formation: $Pu(c,l) + 1.5F_2(g) = PuF_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	22.140	30.141	30.141	0	-371.000	-354.320	259.721
300*	22.173	30.278	30.141	.041	-370.995	-354.218	258.044
395	23.573	36.575	30.957	2.219	-370.717	-348.944	193.065
395	23.573	36.575	30.957	2.219	-371.537	-348.944	193.065
400	23.647	36.872	31.030	2.337	-371.520	-348.659	190.496
480	24.514	41.265	32.378	4.266	-371.218	-344.114	156.677
480	24.514	41.265	32.378	4.266	-371.353	-344.114	156.677
500	24.731	42.270	32.754	4.758	-371.276	-342.981	149.915
588	25.515	46.343	34.489	6.970	-370.935	-338.031	125.639
588	25.515	46.343	34.489	6.970	-371.075	-338.031	125.639
600	25.622	46.860	34.732	7.277	-371.025	-337.356	122.880
700	26.403	50.869	36.756	9.879	-370.583	-331.778	103.585
730	26.617	51.981	37.359	10.674	-370.440	-330.118	98.831
730	26.617	51.981	37.359	10.674	-370.460	-330.118	98.831
752	26.774	52.775	37.799	11.262	-370.345	-328.906	95.587
752	26.774	52.775	37.799	11.262	-370.785	-328.906	95.587
800	27.116	54.442	38.748	12.555	-370.510	-326.242	89.124
900	27.784	57.675	40.675	15.300	-369.894	-320.744	77.886
913	27.867	58.074	40.920	15.662	-369.810	-320.034	76.607
913	27.867	58.074	40.920	15.662	-370.485	-320.034	76.607
1000	28.421	60.635	42.524	18.111	-370.063	-315.246	68.896
1100	29.036	63.373	44.297	20.984	-369.529	-309.789	61.549
1200	29.636	65.926	45.995	23.917	-368.943	-304.386	55.435
1300	30.223	68.321	47.621	26.910	-368.302	-299.030	50.271
1400	30.801	70.582	49.181	29.962	-367.610	-293.728	45.852
1500	31.372	72.726	50.679	33.070	-366.866	-288.476	42.030
1600	31.938	74.769	52.121	36.236	-366.070	-283.274	38.693
1699	32.495	76.703	53.498	39.425	-365.229	-278.176	35.783
1699	35.000	84.355	53.498	52.425	-352.229	-278.176	35.783
1700	35.000	84.375	53.516	52.460	-352.217	-278.132	35.756
1800	35.000	86.376	55.287	55.960	-351.096	-273.809	33.245
1900	35.000	88.268	56.973	59.460	-349.975	-269.544	31.004
2000	35.000	90.064	58.584	62.960	-348.861	-265.342	28.995

*Data above 298 K estimated except temperature of fusion.

Phase changes: 395 K, α - β transition point of Pu; $\Delta H°$ = 0.820 kcal/mol.
480 K, β - γ transition point of Pu; $\Delta H°$ = 0.135 kcal/mol.
588 K, γ - δ transition point of Pu; $\Delta H°$ = 0.140 kcal/mol.
730 K, δ - δ' transition point of Pu; $\Delta H°$ = 0.020 kcal/mol.
752 K, δ' - ε transition point of Pu; $\Delta H°$ = 0.440 kcal/mol.
913 K, melting point of Pu; $\Delta H°$ = 0.675 kcal/mol.
1699 K, melting point of PuF_3; $\Delta H°$ = 13.000 kcal/mol.

PuF_3(c,l) - Continued

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1699 K: $Cp^\circ = 22.657 + 5.894\times10^{-3}T - 2.022\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 22.657\times10^{-3}T + 2.947\times10^{-6}T^2 + 2.022\times10^{2}T^{-1} - 7.695$

1699-2000 K: $Cp^\circ = 35.000$

$H^\circ - H^\circ_{298} = 35.000\times10^{-3}T - 7.040$

Formation equations (kcal/mol):

298.15-395 K: $\Delta Hf^\circ = -372.596 + 5.905\times10^{-3}T - 3.788\times10^{-6}T^2 + 51.450T^{-1}$

$\Delta Gf^\circ = -372.596 - 5.905\times10^{-3}T\ln T + 3.788\times10^{-6}T^2 + 25.725T^{-1} + 93.524\times10^{-3}T$

395-480 K: $\Delta Hf^\circ = -373.207 + 3.838\times10^{-3}T + 0.102\times10^{-6}T^2 + 51.450T^{-1}$

$\Delta Gf^\circ = -373.207 - 3.838\times10^{-3}T\ln T - 0.102\times10^{-6}T^2 + 25.725T^{-1} + 84.247\times10^{-3}T$

480-588 K: $\Delta Hf^\circ = -373.603 + 4.793\times10^{-3}T - 0.756\times10^{-6}T^2 + 51.450T^{-1}$

$\Delta Gf^\circ = -373.603 - 4.793\times10^{-3}T\ln T + 0.756\times10^{-6}T^2 + 25.725T^{-1} + 90.556\times10^{-3}T$

588-730 K: $\Delta Hf^\circ = -372.713 + 1.018\times10^{-3}T + 2.686\times10^{-6}T^2 + 51.450T^{-1}$

$\Delta Gf^\circ = -372.713 - 1.018\times10^{-3}T\ln T - 2.686\times10^{-6}T^2 + 25.725T^{-1} + 66.995\times10^{-3}T$

730-752 K: $\Delta Hf^\circ = -373.008 + 1.395\times10^{-3}T + 2.686\times10^{-6}T^2 + 51.450T^{-1}$

$\Delta Gf^\circ = -373.008 - 1.395\times10^{-3}T\ln T - 2.686\times10^{-6}T^2 + 25.725T^{-1} + 69.885\times10^{-3}T$

752-913 K: $\Delta Hf^\circ = -373.650 + 1.663\times10^{-3}T + 2.686\times10^{-6}T^2 + 51.450T^{-1}$

$\Delta Gf^\circ = -373.650 - 1.663\times10^{-3}T\ln T - 2.686\times10^{-6}T^2 + 25.725T^{-1} + 72.513\times10^{-3}T$

913-1699 K: $\Delta Hf^\circ = -372.619 - 0.205\times10^{-3}T + 2.686\times10^{-6}T^2 + 51.450T^{-1}$

$\Delta Gf^\circ = -372.619 + 0.205\times10^{-3}T\ln T - 2.686\times10^{-6}T^2 + 25.725T^{-1} + 58.650\times10^{-3}T$

1699-2000 K: $\Delta Hf^\circ = -371.964 + 12.138\times10^{-3}T - 0.261\times10^{-6}T^2 - 150.750T^{-1}$

$\Delta Gf^\circ = -371.964 - 12.138\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 - 75.375T^{-1} + 145.097\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Fuger (83). Low-temperature heat capacities and entropy at 298 K from Osborne (177). Oetting (174) estimated data above 298 K except temperatures of fusion. His estimates were adjusted to merge smoothly with low-temperature heat capacities.

$PuF_4(c,l)$

Plutonium Tetrafluoride

[Formation: $Pu(c,l) + 2F_2(g) = PuF_4(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	27.770	35.194	35.194	0	-425.000	-402.605	295.114
300*	27.805	35.366	35.196	.051	-424.992	-402.468	293.194
395	29.197	43.216	36.214	2.766	-424.542	-395.399	218.768
395	29.197	43.216	36.214	2.766	-425.362	-395.399	218.768
400	29.270	43.584	36.304	2.912	-425.336	-395.020	215.826
480	30.007	48.992	37.980	5.286	-424.910	-388.996	177.112
480	30.007	48.992	37.980	5.286	-425.045	-388.996	177.112
500	30.191	50.221	38.445	5.888	-424.939	-387.497	169.373
588	30.761	55.164	40.587	8.571	-424.492	-380.947	141.590
588	30.761	55.164	40.587	8.571	-424.632	-380.947	141.590
600	30.839	55.786	40.884	8.941	-424.570	-380.055	138.433
700	31.331	60.579	43.365	12.050	-424.045	-372.678	116.354
730	31.450	61.896	44.099	12.992	-423.884	-370.480	110.914
730	31.450	61.896	44.099	12.992	-423.904	-370.480	110.914
752	31.537	62.832	44.633	13.686	-423.777	-368.872	107.202
752	31.537	62.832	44.633	13.686	-424.217	-368.872	107.202
800	31.727	64.789	45.784	15.204	-423.924	-365.349	99.807
900	32.057	68.545	48.107	18.394	-423.299	-358.062	86.948
913	32.094	69.005	48.402	18.811	-423.217	-357.120	85.485
913	32.094	69.005	48.402	18.811	-423.892	-357.120	85.485
1000	32.343	71.938	50.324	21.614	-423.499	-350.777	76.661
1100	32.595	75.033	52.432	24.861	-423.034	-343.527	68.252
1200	32.822	77.879	54.436	28.132	-422.555	-336.321	61.252
1300	33.031	80.514	56.341	31.425	-422.062	-329.152	55.335
1310	33.051	80.768	56.527	31.755	-422.013	-328.439	54.793
1310	41.000	88.554	56.527	41.955	-411.813	-328.439	54.793
1400	41.000	91.278	58.674	45.645	-410.652	-322.752	50.383
1500	41.000	94.107	60.944	49.745	-409.368	-316.518	46.116

*Data above 298 K estimated.

Phase changes: 395 K, α - β transition point of Pu; ΔH° = 0.820 kcal/mol.
480 K, β - γ transition point of Pu; ΔH° = 0.135 kcal/mol.
588 K, γ - δ transition point of Pu; ΔH° = 0.140 kcal/mol.
730 K, δ - δ' transition point of Pu; ΔH° = 0.020 kcal/mol.
752 K, δ' - ε transition point of Pu; ΔH° = 0.440 kcal/mol.
913 K, melting point of Pu; ΔH° = 0.675 kcal/mol.
1310 K, melting point of PuF_4; ΔH° = 10.200 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1310 K: $Cp^\circ = 30.013 + 2.554\times10^{-3}T - 2.670\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 30.013\times10^{-3}T + 1.277\times10^{-6}T^2 + 2.670\times10^{2}T^{-1} - 9.957$

1310-1500 K: $Cp^\circ = 41.000$

$H^\circ - H^\circ_{298} = 41.000\times10^{-3}T - 11.755$

PuF_4(c,1) - Continued

Formation equations (kcal/mol):

298.15-395 K: $\Delta Hf^\circ = -427.414 + 9.007\times10^{-3}T - 5.545\times10^{-6}T^2 + 66.000T^{-1}$

$\Delta Gf^\circ = -427.414 - 9.007\times10^{-3}T\ln T + 5.545\times10^{-6}T^2 + 33.000T^{-1} + 132.502\times10^{-3}T$

395-480 K: $\Delta Hf^\circ = -428.024 + 6.940\times10^{-3}T - 1.655\times10^{-6}T^2 + 66.000T^{-1}$

$\Delta Gf^\circ = -428.024 - 6.940\times10^{-3}T\ln T + 1.655\times10^{-6}T^2 + 33.000T^{-1} + 123.226\times10^{-3}T$

480-588 K: $\Delta Hf^\circ = -428.420 + 7.895\times10^{-3}T - 2.513\times10^{-6}T^2 + 66.000T^{-1}$

$\Delta Gf^\circ = -428.420 - 7.895\times10^{-3}T\ln T + 2.513\times10^{-6}T^2 + 33.000T^{-1} + 129.534\times10^{-3}T$

588-730 K: $\Delta Hf^\circ = -427.530 + 4.120\times10^{-3}T + 0.929\times10^{-6}T^2 + 66.000T^{-1}$

$\Delta Gf^\circ = -427.530 - 4.120\times10^{-3}T\ln T - 0.929\times10^{-6}T^2 + 33.000T^{-1} + 105.973\times10^{-3}T$

730-752 K: $\Delta Hf^\circ = -427.826 + 4.497\times10^{-3}T + 0.929\times10^{-6}T^2 + 66.000T^{-1}$

$\Delta Gf^\circ = -427.826 - 4.497\times10^{-3}T\ln T - 0.929\times10^{-6}T^2 + 33.000T^{-1} + 108.863\times10^{-3}T$

752-913 K: $\Delta Hf^\circ = -428.467 + 4.765\times10^{-3}T + 0.929\times10^{-6}T^2 + 66.000T^{-1}$

$\Delta Gf^\circ = -428.467 - 4.765\times10^{-3}T\ln T - 0.929\times10^{-6}T^2 + 33.000T^{-1} + 111.491\times10^{-3}T$

913-1310 K: $\Delta Hf^\circ = -427.437 + 2.897\times10^{-3}T + 0.929\times10^{-6}T^2 + 66.000T^{-1}$

$\Delta Gf^\circ = -427.437 - 2.897\times10^{-3}T\ln T - 0.929\times10^{-6}T^2 + 33.000T^{-1} + 97.629\times10^{-3}T$

1310-1500 K: $\Delta Hf^\circ = -429.234 + 13.884\times10^{-3}T - 0.348\times10^{-6}T^2 - 201.000T^{-1}$

$\Delta Gf^\circ = -429.234 - 13.884\times10^{-3}T\ln T + 0.348\times10^{-6}T^2 - 100.500T^{-1} + 176.268\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Fuger (83). Low-temperature heat capacities and entropy at 298 K from Osborne (178). Oetting (174) estimated data above 298 K. His estimates were adjusted to merge smoothly with low-temperature heat capacities.

$PuF_6(c,l)$

Plutonium Hexafluoride

[Formation: $Pu(c) + 3F_2(g) = PuF_6(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	40.000	53.000	53.000	0	-430.000	-398.471	292.083
300	40.020	53.247	53.000	.074	-429.983	-398.276	290.140
324.74	42.494	56.488	53.144	1.086	-429.730	-395.672	266.283
324.74	45.000	70.210	53.144	5.542	-425.274	-395.672	266.283
335.31	45.000	71.651	53.703	6.018	-425.127	-394.710	257.262

*Heat capacities estimated.

Phase changes: 324.74 K, melting point of PuF_6; ΔH° = 4.456 kcal/mol.
335.31 K, boiling point of PuF_6; ΔH° sublimation at 298 K = 11.6 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-324.74 K: $Cp^\circ = 21.109 + 63.364\times10^{-3}T$

$H^\circ - H^\circ_{298} = 21.109\times10^{-3}T + 31.682\times10^{-6}T^2 - 9.110$

324.74-335.31 K: $Cp^\circ = 45.000$

$H^\circ - H^\circ_{298} = 45.000\times10^{-3}T - 9.071$

Formation equations (kcal/mol):

298.15-324.74 K: $\Delta Hf^\circ = -428.677 - 8.405\times10^{-3}T + 24.686\times10^{-6}T^2 - 301.500T^{-1}$

$\Delta Gf^\circ = -428.677 + 8.405\times10^{-3}T\ln T - 24.686\times10^{-6}T^2 - 150.750T^{-1} + 62.480\times10^{-3}T$

324.74-335.31 K: $\Delta Hf^\circ = -428.639 + 15.486\times10^{-3}T - 6.996\times10^{-6}T^2 - 301.500T^{-1}$

$\Delta Gf^\circ = -428.639 - 15.486\times10^{-3}T\ln T + 6.996\times10^{-6}T^2 - 150.750T^{-1} + 190.235\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Fuger (83). Other data from Oetting (174) who estimated heat capacities.

$PuF_6(g)$

Plutonium Hexafluoride (ideal gas)

[Formation: $Pu(c,l) + 3F_2(g) = PuF_6(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	30.933	88.294	88.294	0	-418.000	-396.994	291.001
300	30.994	88.485	88.295	.057	-418.000	-396.865	289.112
395	33.321	97.353	89.441	3.125	-417.927	-390.180	215.880
395	33.321	97.353	89.441	3.125	-418.747	-390.180	215.880
400	33.444	97.773	89.543	3.292	-418.739	-389.819	212.984
480	34.542	103.981	91.445	6.017	-418.602	-384.047	174.859
480	34.542	103.981	91.445	6.017	-418.737	-384.047	174.859
500	34.816	105.397	91.975	6.711	-418.703	-382.603	167.233
588	35.541	111.105	94.421	9.810	-418.570	-376.263	139.849
588	35.541	111.105	94.421	9.810	-418.710	-376.263	139.849
600	35.640	111.824	94.762	10.237	-418.691	-375.396	136.736
700	36.167	117.360	97.604	13.829	-418.531	-368.192	114.953
730	36.273	118.880	98.448	14.916	-418.482	-366.036	109.584
730	36.273	118.880	98.448	14.916	-418.502	-366.036	109.584
752	36.351	119.960	99.060	15.716	-418.458	-364.456	105.919
752	36.351	119.960	99.060	15.716	-418.898	-364.456	105.919
800	36.521	122.214	100.383	17.465	-418.790	-360.985	98.615
900	36.771	126.531	103.053	21.130	-418.561	-353.771	85.906
913	36.795	127.059	103.391	21.608	-418.532	-352.836	84.459
913	36.795	127.059	103.391	21.608	-419.207	-352.836	84.459
1000	36.952	130.415	105.599	24.816	-419.175	-346.515	75.730
1100	37.088	133.943	108.017	28.519	-419.140	-339.248	67.402
1200	37.192	137.175	110.314	32.233	-419.109	-331.988	60.462
1300	37.274	140.155	112.497	35.956	-419.081	-324.727	54.591
1400	37.340	142.920	114.572	39.687	-419.060	-317.473	49.559
1500	37.392	145.498	116.549	43.424	-419.042	-310.217	45.198
1600	37.436	147.913	118.435	47.165	-419.029	-302.962	41.382
1700	37.472	150.184	120.236	50.911	-419.017	-295.706	38.015
1800	37.502	152.326	121.959	54.660	-419.014	-288.453	35.023
1900	37.528	154.355	123.612	58.411	-419.012	-281.199	32.345
2000	37.550	156.280	125.198	62.165	-419.019	-273.947	29.935

Phase changes: 395 K, α - β transition point of Pu; $\Delta H°$ = 0.820 kcal/mol.
480 K, β - γ transition point of Pu; $\Delta H°$ = 0.135 kcal/mol.
588 K, γ - δ transition point of Pu; $\Delta H°$ = 0.140 kcal/mol.
730 K, δ - δ' transition point of Pu; $\Delta H°$ = 0.020 kcal/mol.
752 K, δ' - ε transition point of PU; $\Delta H°$ = 0.440 kcal/mol.
913 K, melting point of Pu; $\Delta H°$ = 0.675 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 36.674 + 0.672\times10^{-3}T - 5.281\times10^{5}T^{-2}$

$H°- H°_{298} = 36.674\times10^{-3}T + 0.336\times10^{-6}T^{2} + 5.281\times10^{2}T^{-1} - 12.735$

PuF_6(g) - Continued

Formation equations (kcal/mol):

298.15-395 K: $\Delta Hf^\circ = -420.303 + 7.160\times10^{-3}T - 6.660\times10^{-6}T^2 + 226.600T^{-1}$

$\Delta Gf^\circ = -420.303 - 7.160\times10^{-3}T\ln T + 6.660\times10^{-6}T^2 + 113.300T^{-1} + 115.713\times10^{-3}T$

395-480 K: $\Delta Hf^\circ = -420.913 + 5.093\times10^{-3}T - 2.770\times10^{-6}T^2 + 226.600T^{-1}$

$\Delta Gf^\circ = -420.913 - 5.093\times10^{-3}T\ln T + 2.770\times10^{-6}T^2 + 113.300T^{-1} + 106.437\times10^{-3}T$

480-588 K: $\Delta Hf^\circ = -421.309 + 6.048\times10^{-3}T - 3.628\times10^{-6}T^2 + 226.600T^{-1}$

$\Delta Gf^\circ = -421.309 - 6.048\times10^{-3}T\ln T + 3.628\times10^{-6}T^2 + 113.300T^{-1} + 112.745\times10^{-3}T$

588-730 K: $\Delta Hf^\circ = -420.419 + 2.273\times10^{-3}T - 0.186\times10^{-6}T^2 + 226.600T^{-1}$

$\Delta Gf^\circ = -420.419 - 2.273\times10^{-3}T\ln T + 0.186\times10^{-6}T^2 + 113.300T^{-1} + 89.184\times10^{-3}T$

730-752 K: $\Delta Hf^\circ = -420.715 + 2.650\times10^{-3}T - 0.186\times10^{-6}T^2 + 226.600T^{-1}$

$\Delta Gf^\circ = -420.715 - 2.650\times10^{-3}T\ln T + 0.186\times10^{-6}T^2 + 113.300T^{-1} + 92.074\times10^{-3}T$

752-913 K: $\Delta Hf^\circ = -421.356 + 2.918\times10^{-3}T - 0.186\times10^{-6}T^2 + 226.600T^{-1}$

$\Delta Gf^\circ = -421.356 - 2.918\times10^{-3}T\ln T + 0.186\times10^{-6}T^2 + 113.300T^{-1} + 94.702\times10^{-3}T$

913-2000 K: $\Delta Hf^\circ = -420.326 + 1.050\times10^{-3}T - 0.186\times10^{-6}T^2 + 226.600T^{-1}$

$\Delta Gf^\circ = -420.326 - 1.050\times10^{-3}T\ln T + 0.186\times10^{-6}T^2 + 113.300T^{-1} + 80.840\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Fuger (83). Other data from Oetting (174).

$PuI_3(c,l)$

Plutonium Triiodide

[Formation: $Pu(c,l) + 1.5I_2(c,l,g) = PuI_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	26.730	51.200	51.200	0	-138.600	-137.450	100.752
300	26.740	51.365	51.202	.049	-138.602	-137.443	100.126
386.8	27.226	58.210	52.036	2.388	-138.805	-137.088	77.456
386.8	27.226	58.210	52.036	2.388	-144.369	-137.088	77.456
395	27.272	58.782	52.170	2.612	-144.459	-136.933	75.763
395	27.272	58.782	52.170	2.612	-145.279	-136.933	75.763
400	27.300	59.125	52.255	2.748	-145.328	-136.827	74.758
458.4	27.545	62.854	53.374	4.345	-145.901	-135.543	64.622
458.4	27.545	62.854	53.374	4.345	-160.932	-135.543	64.622
480	27.636	64.124	53.829	4.941	-160.809	-134.347	61.169
480	27.636	64.124	53.829	4.941	-160.944	-134.347	61.169
500	27.720	65.254	54.264	5.495	-160.829	-133.242	58.239
588	28.151	69.782	56.255	7.954	-160.332	-128.429	47.734
588	28.151	69.782	56.255	7.954	-160.472	-128.429	47.734
600	28.210	70.351	56.531	8.292	-160.402	-127.775	46.541
700	28.700	74.736	58.826	11.137	-159.793	-122.385	38.210
730	28.850	75.944	59.505	12.000	-159.601	-120.786	36.161
730	28.850	75.944	59.505	12.000	-159.621	-120.786	36.161
752	28.960	76.803	59.999	12.636	-159.469	-119.617	34.763
752	28.960	76.803	59.999	12.636	-159.909	-119.617	34.763
800	29.200	78.602	61.062	14.032	-159.559	-117.056	31.978
900	29.690	82.069	63.206	16.977	-158.793	-111.790	27.146
913	29.754	82.495	63.477	17.363	-158.690	-111.111	26.597
913	29.754	82.495	63.477	17.363	-159.365	-111.111	26.597
1000	30.180	85.223	65.253	19.970	-158.817	-106.537	23.283
1050	30.420	86.701	66.239	21.485	-158.487	-103.933	21.633
1050	34.000	98.130	66.239	33.485	-146.487	-103.933	21.633
1100	34.000	99.711	67.725	35.185	-145.973	-101.918	20.249
1200	34.000	102.670	70.516	38.585	-144.946	-97.959	17.841
1300	34.000	105.391	73.095	41.985	-143.920	-94.084	15.817
1400	34.000	107.911	75.493	45.385	-142.898	-90.288	14.094
1500	34.000	110.257	77.734	48.785	-141.877	-86.568	12.613

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
395 K, α - β transition point of Pu; $\Delta H°$ = 0.820 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
480 K, β - γ transition point of Pu; $\Delta H°$ = 0.135 kcal/mol.
588 K, γ - δ transition point of Pu; $\Delta H°$ = 0.140 kcal/mol.
730 K, δ - δ' transition point of Pu; $\Delta H°$ = 0.020 kcal/mol.
752 K, δ' - ε transition point of Pu; $\Delta H°$ = 0.440 kcal/mol.
913 K, melting point of Pu; $\Delta H°$ = 0.675 kcal/mol.
1050 K, melting point of PuI_3; $\Delta H°$ = 12.000 kcal/mol.

PuI_3(c,1) - Continued

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1050 K: $Cp^\circ = 25.260 + 4.920\times10^{-3}T$

$H^\circ - H^\circ_{298} = 25.260\times10^{-3}T + 2.460\times10^{-6}T^2 - 7.750$

1050-1500 K: $Cp^\circ = 34.000$

$H^\circ - H^\circ_{298} = 34.000\times10^{-3}T - 2.215$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -138.627 + 1.954\times10^{-3}T - 6.252\times10^{-6}T^2$

$\Delta Gf^\circ = -138.627 - 1.954\times10^{-3}T\ln T + 6.252\times10^{-6}T^2 + 13.219\times10^{-3}T$

386.8-395 K: $\Delta Hf^\circ = -140.810 - 7.652\times10^{-3}T - 4.014\times10^{-6}T^2$

$\Delta Gf^\circ = -140.810 + 7.652\times10^{-3}T\ln T + 4.014\times10^{-6}T^2 - 37.503\times10^{-3}T$

395-458.4 K: $\Delta Hf^\circ = -141.420 - 9.719\times10^{-3}T - 0.124\times10^{-6}T^2$

$\Delta Gf^\circ = -141.420 + 9.719\times10^{-3}T\ln T + 0.124\times10^{-6}T^2 - 46.780\times10^{-3}T$

458.4-480 K: $\Delta Hf^\circ = -163.490 + 5.792\times10^{-3}T - 0.226\times10^{-6}T^2 - 22.950T^{-1}$

$\Delta Gf^\circ = -163.490 - 5.792\times10^{-3}T\ln T + 0.226\times10^{-6}T^2 - 11.475T^{-1} + 96.415\times10^{-3}T$

480-588 K: $\Delta Hf^\circ = -163.886 + 6.746\times10^{-3}T - 1.084\times10^{-6}T^2 - 22.950T^{-1}$

$\Delta Gf^\circ = -163.886 - 6.746\times10^{-3}T\ln T + 1.084\times10^{-6}T^2 - 11.475T^{-1} + 102.723\times10^{-3}T$

588-730 K: $\Delta Hf^\circ = -162.996 + 2.972\times10^{-3}T + 2.358\times10^{-6}T^2 - 22.950T^{-1}$

$\Delta Gf^\circ = -162.996 - 2.972\times10^{-3}T\ln T - 2.358\times10^{-6}T^2 - 11.475T^{-1} + 79.162\times10^{-3}T$

730-752 K: $\Delta Hf^\circ = -163.291 + 3.348\times10^{-3}T + 2.358\times10^{-6}T^2 - 22.950T^{-1}$

$\Delta Gf^\circ = -163.291 - 3.348\times10^{-3}T\ln T - 2.358\times10^{-6}T^2 - 11.475T^{-1} + 82.052\times10^{-3}T$

752-913 K: $\Delta Hf^\circ = -163.933 + 3.616\times10^{-3}T + 2.358\times10^{-6}T^2 - 22.950T^{-1}$

$\Delta Gf^\circ = -163.933 - 3.616\times10^{-3}T\ln T - 2.358\times10^{-6}T^2 - 11.475T^{-1} + 84.680\times10^{-3}T$

913-1050 K: $\Delta Hf^\circ = -162.902 + 1.748\times10^{-3}T + 2.358\times10^{-6}T^2 - 22.950T^{-1}$

$\Delta Gf^\circ = -162.902 - 1.748\times10^{-3}T\ln T - 2.358\times10^{-6}T^2 - 11.475T^{-1} + 70.817\times10^{-3}T$

1050-1500 K: $\Delta Hf^\circ = -157.367 + 10.489\times10^{-3}T - 0.102\times10^{-6}T^2 - 22.950T^{-1}$

$\Delta Gf^\circ = -157.367 - 10.489\times10^{-3}T\ln T + 0.102\times10^{-6}T^2 - 11.475T^{-1} + 123.763\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Brown (19). Other data are those estimated by Oetting (174).

RbCl(g)

Rubidium Chloride (ideal gas)

[Formation: $Rb(c,l,g) + 0.5Cl_2(g)] = RbCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.814	59.664	59.664	0	-54.700	-59.074	43.302
300	8.816	59.719	59.666	.016	-54.706	-59.101	43.055
312.64	8.829	60.083	59.675	.128	-54.741	-59.286	41.443
312.64	8.829	60.083	59.675	.128	-55.265	-59.286	41.443
400	8.915	62.270	60.013	.903	-55.556	-60.370	32.984
500	8.973	64.266	60.670	1.798	-55.855	-61.540	26.899
600	9.014	65.905	61.410	2.697	-56.128	-62.651	22.820
700	9.046	67.297	62.154	3.600	-56.379	-63.718	19.893
800	9.075	68.507	62.875	4.506	-56.615	-64.751	17.689
900	9.100	69.578	63.561	5.415	-56.840	-65.747	15.965
974.5	9.118	70.302	64.050	6.093	-57.010	-66.482	14.910
974.5	9.118	70.302	64.050	6.093	-74.240	-66.482	14.910
1000	9.124	70.538	64.212	6.326	-74.249	-66.280	14.485
1100	9.147	71.409	64.827	7.240	-74.280	-65.481	13.010
1200	9.170	72.205	65.408	8.156	-74.311	-64.679	11.779
1300	9.192	72.940	65.960	9.074	-74.340	-63.874	10.738
1400	9.213	73.622	66.483	9.994	-74.369	-63.068	9.845
1500	9.234	74.259	66.981	10.917	-74.396	-62.260	9.071
1600	9.255	74.855	67.454	11.841	-74.424	-61.450	8.394
1700	9.276	75.417	67.906	12.768	-74.450	-60.638	7.795
1800	9.296	75.948	68.339	13.696	-74.475	-59.826	7.264
1900	9.317	76.451	68.753	14.627	-74.500	-59.010	6.788
2000	9.337	76.929	69.149	15.560	-74.527	-58.195	6.359

Phase changes: 312.64 K, melting point of Rb; ΔH° = 0.524 kcal/mol.
974.5 K, boiling point of Rb to monatomic gas; ΔH° = 17.230 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.935 + 0.204\times10^{-3}T - 0.162\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.935\times10^{-3}T + 0.102\times10^{-6}T^2 + 0.162\times10^{2}T^{-1} - 2.727$

Formation equations (kcal/mol):

298.15-312.64 K: $\Delta Hf^\circ = -54.807 + 3.989\times10^{-3}T - 11.498\times10^{-6}T^2 - 17.950T^{-1}$

$\Delta Gf^\circ = -54.807 - 3.989\times10^{-3}T\ln T + 11.498\times10^{-6}T^2 - 8.975T^{-1} + 5.087\times10^{-3}T$

312.64-974.5 K: $\Delta Hf^\circ = -54.462 - 3.352\times10^{-3}T + 0.696\times10^{-6}T^2 + 55.250T^{-1}$

$\Delta Gf^\circ = -54.462 + 3.352\times10^{-3}T\ln T - 0.696\times10^{-6}T^2 + 27.625T^{-1} - 34.746\times10^{-3}T$

974.5-2000 K: $\Delta Hf^\circ = -73.804 - 0.468\times10^{-3}T + 0.060\times10^{-6}T^2 - 35.850T^{-1}$

$\Delta Gf^\circ = -73.804 + 0.468\times10^{-3}T\ln T - 0.060\times10^{-6}T^2 - 17.925T^{-1} + 4.371\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data from Wilkens (265).

RbF(c,l)

Rubidium Fluoride

[Formation: $Rb(c,l,g) + 0.5F_2(g) = RbF(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	12.040	19.200	19.200	0	-133.300	-126.332	92.603
300	12.058	19.275	19.202	.022	-133.299	-126.289	92.001
312.64	12.161	19.775	19.215	.175	-133.289	-125.994	88.075
312.64	12.161	19.775	19.215	.175	-133.813	-125.994	88.075
400	12.875	22.867	19.685	1.273	-133.755	-123.813	67.647
500	13.468	25.806	20.624	2.591	-133.607	-121.346	53.040
600	13.986	28.308	21.701	3.964	-133.385	-118.913	43.314
700	14.468	30.501	22.805	5.387	-133.102	-116.523	36.380
800	14.931	32.463	23.892	6.857	-132.762	-114.177	31.191
900	15.383	34.248	24.945	8.373	-132.371	-111.869	27.165
974.5	15.715	35.485	25.703	9.532	-132.055	-110.189	24.712
974.5	15.715	35.485	25.703	9.532	-149.285	-110.189	24.712
1000	15.828	35.892	25.958	9.934	-149.122	-109.169	23.858
1068	16.129	36.943	26.625	11.020	-148.675	-106.466	21.786
1068	17.000	42.678	26.625	17.145	-142.550	-106.466	21.786
1100	17.000	43.179	27.098	17.689	-142.307	-105.388	20.938
1200	17.000	44.659	28.502	19.389	-141.549	-102.066	18.589
1300	17.000	46.019	29.797	21.089	-140.793	-98.804	16.610
1400	17.000	47.279	31.001	22.789	-140.040	-95.604	14.924

*Heat capacity at 298 K estimated.

Phase changes: 312.64 K, melting point of Rb; ΔH° = 0.524 kcal/mol.
974.5 K, boiling point of Rb to monatomic gas; ΔH° = 17.230 kcal/mol.
1068 K, melting point of RbF; ΔH° = 6.125 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1068 K: $Cp^\circ = 11.622 + 4.280\times10^{-3}T - 0.735\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 11.622\times10^{-3}T + 2.140\times10^{-6}T^2 + 0.735\times10^{2}T^{-1} - 3.902$

1068-1400 K: $Cp^\circ = 17.000$

$H^\circ - H^\circ_{298} = 17.000\times10^{-3}T - 1.011$

Formation equations (kcal/mol):

298.15-312.64 K: $\Delta Hf^\circ = -134.571 + 6.835\times10^{-3}T - 9.503\times10^{-6}T^2 + 23.250T^{-1}$

$\Delta Gf^\circ = -134.571 - 6.835\times10^{-3}T\ln T + 9.503\times10^{-6}T^2 + 11.625T^{-1} + 63.614\times10^{-3}T$

312.64-974.5 K: $\Delta Hf^\circ = -134.226 - 0.505\times10^{-3}T + 2.691\times10^{-6}T^2 + 96.450T^{-1}$

$\Delta Gf^\circ = -134.226 + 0.505\times10^{-3}T\ln T - 2.691\times10^{-6}T^2 + 48.225T^{-1} + 23.780\times10^{-3}T$

974.5-1068 K: $\Delta Hf^\circ = -153.568 + 2.378\times10^{-3}T + 2.055\times10^{-6}T^2 + 5.350T^{-1}$

$\Delta Gf^\circ = -153.568 - 2.378\times10^{-3}T\ln T - 2.055\times10^{-6}T^2 + 2.675T^{-1} + 62.897\times10^{-3}T$

1068-1400 K: $\Delta Hf^\circ = -150.677 + 7.756\times10^{-3}T - 0.085\times10^{-6}T^2 - 68.150T^{-1}$

$\Delta Gf^\circ = -150.677 - 7.756\times10^{-3}T\ln T + 0.085\times10^{-6}T^2 - 34.075T^{-1} + 95.441\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Entropy at 298 K from Kelley (118). High-temperature data based on Macleod (149). Heat capacity at 298 K estimated by Macleod (149).

SCl(g)

Sulfur Monochloride (ideal gas)

[Reaction: $0.5S_2(g) + 0.5Cl_2(g) = SCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15*	8.973	56.696	56.696	0	22.045	21.211	-15.548
300	8.977	56.751	56.696	.017	22.048	21.206	-15.449
400	9.100	59.355	57.050	.922	22.139	20.911	-11.425
500	9.116	61.388	57.722	1.833	22.210	20.596	-9.002
600	9.108	63.050	58.477	2.744	22.262	20.267	-7.382
700	9.099	64.453	59.232	3.655	22.304	19.932	-6.223
800	9.091	65.667	59.962	4.564	22.334	19.590	-5.352
900	9.087	66.738	60.657	5.473	22.358	19.245	-4.673
1000	9.085	67.695	61.313	6.382	22.377	18.899	-4.130
1100	9.085	68.561	61.934	7.290	22.389	18.550	-3.686
1200	9.087	69.352	62.519	8.199	22.397	18.201	-3.315
1300	9.090	70.079	63.073	9.108	22.400	17.851	-3.001
1400	9.094	70.753	63.598	10.017	22.399	17.501	-2.732
1500	9.099	71.380	64.096	10.926	22.392	17.152	-2.499
1600	9.104	71.968	64.570	11.837	22.384	16.802	-2.295
1700	9.110	72.520	65.022	12.747	22.370	16.454	-2.115
1800	9.117	73.041	65.453	13.659	22.355	16.107	-1.956
1900	9.124	73.534	65.865	14.571	22.335	15.761	-1.813
2000	9.131	74.002	66.260	15.483	22.311	15.415	-1.684

*Data estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 9.204 - 0.068\times10^{-3}T - 0.188\times10^{5}T^{-2}$

$H°- H°_{298} = 9.204\times10^{-3}T - 0.034\times10^{-6}T^{2} + 0.188\times10^{2}T^{-1} - 2.804$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr° = 22.048 + 0.619\times10^{-3}T - 0.238\times10^{-6}T^{2} - 49.500T^{-1}$

$\Delta Gr° = 22.048 - 0.619\times10^{-3}T\ln T + 0.238\times10^{-6}T^{2} - 24.750T^{-1} + 0.927\times10^{-3}T$

Source: Data are those estimated by Chase (24).

$SCl_2(g)$

Sulfur Dichloride (ideal gas)

[Reaction: $0.5S_2(g) + Cl_2(g) = SCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	12.164	67.285	67.285	0	-19.555	-15.602	11.437
300	12.180	67.360	67.285	.023	-19.554	-15.577	11.348
400	12.821	70.962	67.772	1.276	-19.530	-14.256	7.789
500	13.173	73.864	68.710	2.577	-19.495	-12.940	5.656
600	13.382	76.286	69.776	3.906	-19.459	-11.633	4.237
700	13.515	78.360	70.859	5.251	-19.423	-10.332	3.226
800	13.604	80.170	71.911	6.607	-19.389	-9.035	2.468
900	13.666	81.777	72.920	7.971	-19.354	-7.744	1.880
1000	13.711	83.219	73.879	9.340	-19.323	-6.455	1.411
1100	13.745	84.527	74.788	10.713	-19.295	-5.169	1.027
1200	13.771	85.725	75.651	12.089	-19.270	-3.887	.708
1300	13.791	86.828	76.469	13.467	-19.248	-2.607	.438
1400	13.807	87.850	77.245	14.847	-19.231	-1.326	.207
1500	13.821	88.803	77.984	16.228	-19.218	-.048	.007
1600	13.831	89.696	78.689	17.611	-19.208	1.229	-.168
1700	13.840	90.534	79.360	18.995	-19.203	2.509	-.323
1800	13.848	91.326	80.004	20.379	-19.201	3.784	-.459
1900	13.854	92.075	80.620	21.764	-19.204	5.062	-.582
2000	13.860	92.785	81.210	23.150	-19.211	6.341	-.693

Phase change: 329.94 K, boiling point of SCl_2; $\Delta H° = 7.4$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.671 + 0.144\times10^{-3}T - 1.378\times10^{5}T^{-2}$

$H°- H°_{298} = 13.671\times10^{-3}T + 0.072\times10^{-6}T^{2} + 1.378\times10^{2}T^{-1} - 4.545$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr° = -19.858 + 0.672\times10^{-3}T - 0.176\times10^{-6}T^{2} + 35.350T^{-1}$

$\Delta Gr° = -19.858 - 0.672\times10^{-3}T\ln T + 0.176\times10^{-6}T^{2} + 17.675T^{-1} + 17.856\times10^{-3}T$

Source: Data from Chase (24).

$S_2Cl(g)$

Chlorosulfanyl Radical (ideal gas)

[Reaction: $S_2(g) + 0.5Cl_2(g) = S_2Cl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15*	12.178	69.799	69.799	0	-11.910	-8.525	6.249
300	12.194	69.875	69.799	.023	-11.908	-8.503	6.195
400	12.829	73.479	70.286	1.277	-11.868	-7.376	4.030
500	13.179	76.383	71.225	2.579	-11.819	-6.258	2.735
600	13.386	78.806	72.293	3.908	-11.772	-5.151	1.876
700	13.518	80.880	73.374	5.254	-11.726	-4.050	1.265
800	13.606	82.691	74.429	6.610	-11.685	-2.956	.808
900	13.668	84.297	75.437	7.974	-11.645	-1.868	.454
1000	13.713	85.740	76.397	9.343	-11.610	-.784	.171
1100	13.746	87.048	77.306	10.716	-11.581	.297	-.059
1200	13.772	88.246	78.169	12.092	-11.557	1.375	-.250
1300	13.792	89.349	78.987	13.470	-11.539	2.452	-.412
1400	13.808	90.371	79.763	14.851	-11.527	3.530	-.551
1500	13.821	91.325	80.504	16.232	-11.523	4.603	-.671
1600	13.832	92.217	81.208	17.615	-11.525	5.679	-.776
1700	13.841	93.056	81.881	18.998	-11.535	6.754	-.868
1800	13.848	93.847	82.523	20.383	-11.550	7.832	-.951
1900	13.855	94.596	83.139	21.768	-11.572	8.909	-1.025
2000	13.860	95.307	83.730	23.154	-11.601	9.988	-1.091

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.672 + 0.144\times10^{-3}T - 1.366\times10^{5}T^{-2}$

$H°- H°_{298} = 13.672\times10^{-3}T + 0.072\times10^{-6}T^{2} + 1.366\times10^{2}T^{-1} - 4.541$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr° = -12.272 + 0.915\times10^{-3}T - 0.292\times10^{-6}T^{2} + 34.150T^{-1}$

$\Delta Gr° = -12.272 - 0.915\times10^{-3}T\ln T + 0.292\times10^{-6}T^{2} + 17.075T^{-1} + 17.502\times10^{-3}T$

Source: Data from Chase (24) who estimated all except enthalpy of formation at 298 K.

$S_2Cl_2(g)$
Dichlorodisulfane (ideal gas)
[Reaction: $S_2(g) + Cl_2(g) = S_2Cl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	17.392	78.180	78.180	0	-34.710	-25.880	18.970
300	17.419	78.288	78.181	.032	-34.707	-25.825	18.813
400	18.411	83.445	78.878	1.827	-34.540	-22.890	12.506
500	18.965	87.617	80.221	3.698	-34.349	-19.997	8.741
600	19.316	91.107	81.752	5.613	-34.151	-17.146	6.245
700	19.560	94.104	83.308	7.557	-33.946	-14.328	4.473
800	19.739	96.728	84.826	9.522	-33.738	-11.540	3.153
900	19.871	99.061	86.280	11.503	-33.527	-8.779	2.132
1000	19.964	101.160	87.665	13.495	-33.316	-6.041	1.320
1100	20.024	103.065	88.979	15.495	-33.108	-3.322	.660
1200	20.060	104.809	90.227	17.499	-32.906	-.624	.114
1300	20.074	106.416	91.411	19.506	-32.710	2.057	-.346
1400	20.069	107.903	92.537	21.513	-32.524	4.726	-.738
1500	20.053	109.287	93.607	23.520	-32.347	7.381	-1.075

Phase change: 410.23 K, boiling point of S_2Cl_2; ΔH° = 8.6 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp^\circ = 19.397 + 0.706\times10^{-3}T - 1.969\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.397\times10^{-3}T + 0.353\times10^{-6}T^2 + 1.969\times10^{2}T^{-1} - 6.475$

Reaction equations (kcal/mol):

298.15-1500 K: $\Delta Hr^\circ = -35.571 + 2.227\times10^{-3}T - 0.055\times10^{-6}T^2 + 60.300T^{-1}$

$\Delta Gr^\circ = -35.571 - 2.227\times10^{-3}T\ln T + 0.055\times10^{-6}T^2 + 30.150T^{-1} + 44.838\times10^{-3}T$

Source: Data from Chase (24).

SF(g)

Sulfur Monofluoride (ideal gas)

[Reaction: $0.5S_2(g) + 0.5F_2(g) = SF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	8.401	53.815	53.815	0	-12.255	-12.953	9.495
300	8.407	53.867	53.815	.016	-12.253	-12.956	9.439
400	8.617	56.317	54.147	.868	-12.185	-13.202	7.213
500	8.737	58.254	54.782	1.736	-12.132	-13.463	5.885
600	8.813	59.854	55.497	2.614	-12.093	-13.733	5.002
700	8.864	61.217	56.220	3.498	-12.063	-14.009	4.374
800	8.902	62.403	56.921	4.386	-12.042	-14.289	3.903
900	8.931	63.453	57.589	5.278	-12.025	-14.570	3.538
1000	8.955	64.396	58.224	6.172	-12.015	-14.855	3.247
1100	8.974	65.250	58.824	7.069	-12.009	-15.138	3.008
1200	8.991	66.032	59.393	7.967	-12.007	-15.423	2.809
1300	9.007	66.752	59.931	8.867	-12.009	-15.708	2.641
1400	9.020	67.420	60.443	9.768	-12.017	-15.992	2.497
1500	9.033	68.043	60.929	10.671	-12.027	-16.277	2.371
1600	9.045	68.626	61.392	11.575	-12.041	-16.558	2.262
1700	9.056	69.175	61.834	12.480	-12.060	-16.840	2.165
1800	9.067	69.693	62.256	13.386	-12.082	-17.121	2.079
1900	9.077	70.183	62.660	14.293	-12.107	-17.399	2.001
2000	9.087	70.649	63.049	15.201	-12.136	-17.678	1.932

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.853 + 0.134\times10^{-3}T - 0.438\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.853\times10^{-3}T + 0.067\times10^{-6}T^2 + 0.438\times10^{2}T^{-1} - 2.792$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr^\circ = -12.230 + 0.427\times10^{-3}T - 0.180\times10^{-6}T^2 - 40.600T^{-1}$

$\Delta Gr^\circ = -12.230 - 0.427\times10^{-3}T\ln T + 0.180\times10^{-6}T^2 - 20.300T^{-1} + 0.187\times10^{-3}T$

Source: Data from Chase (26).

$SF_2(g)$

Sulfur Difluoride (ideal gas)

[Reaction: $0.5S_2(g) + F_2(g) = SF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15*	10.733	61.565	61.565	0	-86.255	-82.042	60.138
300	10.753	61.632	61.565	.020	-86.256	-82.016	59.748
400	11.686	64.862	62.000	1.145	-86.299	-80.595	44.034
500	12.307	67.541	62.847	2.347	-86.314	-79.166	34.603
600	12.717	69.824	63.826	3.599	-86.317	-77.737	28.315
700	12.995	71.806	64.826	4.886	-86.308	-76.307	23.824
800	13.188	73.555	65.811	6.195	-86.297	-74.880	20.456
900	13.328	75.117	66.759	7.522	-86.281	-73.453	17.837
1000	13.432	76.526	67.666	8.860	-86.266	-72.028	15.742
1100	13.511	77.810	68.531	10.207	-86.253	-70.605	14.028
1200	13.572	78.989	69.355	11.561	-86.241	-69.184	12.600
1300	13.620	80.077	70.138	12.921	-86.230	-67.762	11.392
1400	13.658	81.088	70.884	14.285	-86.225	-66.343	10.356
1500	13.690	82.031	71.596	15.652	-86.223	-64.923	9.459
1600	13.716	82.916	72.277	17.023	-86.223	-63.503	8.674
1700	13.738	83.748	72.927	18.395	-86.229	-62.083	7.981
1800	13.756	84.534	73.551	19.770	-86.238	-60.662	7.365
1900	13.771	85.278	74.148	21.147	-86.249	-59.240	6.814
2000	13.785	85.985	74.723	22.524	-86.268	-57.819	6.318

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 12.941 + 0.578\times10^{-3}T - 2.116\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 12.941\times10^{-3}T + 0.289\times10^{-6}T^2 + 2.116\times10^{2}T^{-1} - 4.594$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr^\circ = -86.587 + 0.261\times10^{-3}T - 0.045\times10^{-6}T^2 + 76.950T^{-1}$

$\Delta Gr^\circ = -86.587 - 0.261\times10^{-3}T\ln T + 0.045\times10^{-6}T^2 + 38.475T^{-1} + 16.288\times10^{-3}T$

Source: Data from Chase (26) who estimated all except enthalpy of formation at 298 K.

$SF_3(g)$

Sulfur Trifluoride (ideal gas)

[Reaction: $0.5S_2(g) + 1.5F_2(g) = SF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15*	13.773	66.347	66.347	0	-135.755	-125.746	92.173
300	13.813	66.432	66.347	.026	-135.757	-125.683	91.559
400	15.588	70.666	66.913	1.501	-135.835	-122.312	66.827
500	16.769	74.280	68.034	3.123	-135.832	-118.929	51.983
600	17.554	77.411	69.341	4.842	-135.782	-115.553	42.090
700	18.088	80.160	70.694	6.626	-135.701	-112.188	35.026
800	18.463	82.601	72.034	8.454	-135.601	-108.837	29.732
900	18.734	84.792	73.331	10.315	-135.486	-105.496	25.618
1000	18.936	86.777	74.578	12.199	-135.366	-102.172	22.329
1100	19.089	88.589	75.771	14.100	-135.242	-98.858	19.641
1200	19.208	90.256	76.909	16.016	-135.113	-95.556	17.403
1300	19.302	91.797	77.996	17.941	-134.985	-92.264	15.511
1400	19.378	93.230	79.034	19.875	-134.859	-88.984	13.891
1500	19.440	94.569	80.025	21.816	-134.735	-85.712	12.488
1600	19.491	95.826	80.974	23.763	-134.613	-82.448	11.262
1700	19.533	97.009	81.883	25.714	-134.493	-79.190	10.180
1800	19.569	98.126	82.754	27.669	-134.378	-75.940	9.220
1900	19.599	99.185	83.591	29.628	-134.264	-72.695	8.362
2000	19.625	100.191	84.396	31.589	-134.157	-69.459	7.590

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 17.955 + 1.138\times10^{-3}T - 4.019\times10^{5}T^{-2}$

$H°- H°_{298} = 17.955\times10^{-3}T + 0.569\times10^{-6}T^{2} + 4.019\times10^{2}T^{-1} - 6.752$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr° = -136.801 + 1.021\times10^{-3}T + 0.148\times10^{-6}T^{2} + 217.000T^{-1}$

$\Delta Gr° = -136.801 - 1.021\times10^{-3}T\ln T - 0.148\times10^{-6}T^{2} + 108.500T^{-1} + 41.721\times10^{-3}T$

Source: Data from Chase (26) who estimated all except enthalpy of formation at 298 K.

$SF_4(g)$

Sulfur Tetrafluoride (ideal gas)

[Reaction: $0.5S_2(g) + 2F_2(g) = SF_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	18.546	71.590	71.590	0	-197.755	-182.088	133.472
300	18.600	71.704	71.591	.034	-197.756	-181.991	132.578
400	20.912	77.398	72.351	2.019	-197.708	-176.738	96.564
500	22.348	82.231	73.855	4.188	-197.560	-171.510	74.966
600	23.265	86.393	75.606	6.472	-197.360	-166.319	60.581
700	23.874	90.028	77.412	8.831	-197.128	-161.164	50.317
800	24.295	93.245	79.195	11.240	-196.878	-156.044	42.629
900	24.597	96.125	80.918	13.686	-196.614	-150.954	36.656
1000	24.819	98.729	82.572	16.157	-196.347	-145.897	31.885
1100	24.987	101.102	84.149	18.648	-196.076	-140.863	27.987
1200	25.117	103.282	85.654	21.153	-195.803	-135.857	24.743
1300	25.219	105.297	87.089	23.670	-195.531	-130.872	22.001
1400	25.302	107.169	88.458	26.196	-195.264	-125.910	19.655
1500	25.368	108.917	89.764	28.730	-194.997	-120.966	17.624
1600	25.423	110.556	91.012	31.270	-194.735	-116.037	15.850
1700	25.469	112.099	92.208	33.814	-194.477	-111.126	14.286
1800	25.508	113.556	93.354	36.363	-194.224	-106.231	12.898
1900	25.541	114.936	94.454	38.916	-193.972	-101.348	11.658
2000	25.569	116.246	95.511	41.471	-193.730	-96.480	10.543

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 23.999 + 1.094\times10^{-3}T - 5.137\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 23.999\times10^{-3}T + 0.547\times10^{-6}T^2 + 5.137\times10^{2}T^{-1} - 8.927$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr^\circ = -199.531 + 2.811\times10^{-3}T + 0.039\times10^{-6}T^2 + 278.550T^{-1}$

$\Delta Gr^\circ = -199.531 - 2.811\times10^{-3}T\ln T - 0.039\times10^{-6}T^2 + 139.275T^{-1} + 72.969\times10^{-3}T$

Source: Data from Chase (26).

$SF_5(g)$

Sulfur Pentafluoride (ideal gas)

[Reaction: $0.5S_2(g) + 2.5F_2(g) = SF_5(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15*	21.425	72.811	72.811	0	-232.455	-209.930	153.881
300	21.507	72.944	72.811	.040	-232.457	-209.790	152.830
400	24.955	79.646	73.701	2.378	-232.441	-202.230	110.492
500	27.021	85.456	75.486	4.985	-232.257	-194.696	85.100
600	28.309	90.505	77.578	7.756	-231.985	-187.210	68.190
700	29.152	94.936	79.747	10.632	-231.660	-179.772	56.127
800	29.729	98.869	81.897	13.578	-231.304	-172.384	47.093
900	30.139	102.396	83.983	16.572	-230.928	-165.041	40.077
1000	30.440	105.587	85.985	19.602	-230.541	-157.742	34.474
1100	30.667	108.500	87.902	22.658	-230.148	-150.480	29.897
1200	30.842	111.176	89.731	25.734	-229.750	-143.255	26.090
1300	30.982	113.650	91.477	28.825	-229.351	-136.062	22.874
1400	31.095	115.951	93.145	31.929	-228.956	-128.904	20.123
1500	31.190	118.099	94.736	35.044	-228.560	-121.771	17.742
1600	31.271	120.115	96.261	38.167	-228.168	-114.663	15.662
1700	31.342	122.013	97.721	41.297	-227.777	-107.580	13.830
1800	31.406	123.806	99.120	44.435	-227.391	-100.521	12.205
1900	31.466	125.506	100.465	47.578	-227.006	-93.483	10.753
2000	31.522	127.121	101.757	50.728	-226.627	-86.465	9.448

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 29.716 + 1.224\times10^{-3}T - 7.694\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 29.716\times10^{-3}T + 0.612\times10^{-6}T^2 + 7.694\times10^{2}T^{-1} - 11.495$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr^\circ = -235.354 + 4.274\times10^{-3}T + 0.017\times10^{-6}T^2 + 484.000T^{-1}$

$\Delta Gr^\circ = -235.354 - 4.274\times10^{-3}T\ln T - 0.017\times10^{-6}T^2 + 242.000T^{-1} + 106.911\times10^{-3}T$

Source: Data from Chase (24) who estimated all except enthalpy of formation at 298 K.

$SF_6(g)$

Sulfur Hexafluoride (ideal gas)

[Reaction: $0.5S_2(g) + 3F_2(g) = SF_6(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	23.174	69.651	69.651	0	-307.055	-276.366	202.579
300	23.278	69.795	69.652	.043	-307.061	-276.176	201.192
400	27.813	77.162	70.625	2.615	-307.195	-265.851	145.252
500	30.676	83.700	72.600	5.550	-307.086	-255.523	111.688
600	32.521	89.468	74.941	8.716	-306.833	-245.235	89.325
700	33.754	94.580	77.389	12.034	-306.490	-234.994	73.367
800	34.609	99.146	79.827	15.455	-306.091	-224.808	61.414
900	35.223	103.260	82.207	18.948	-305.651	-214.671	52.129
1000	35.676	106.996	84.502	22.494	-305.188	-204.591	44.713
1100	36.020	110.413	86.704	26.080	-304.708	-194.551	38.653
1200	36.286	113.559	88.813	29.695	-304.217	-184.560	33.613
1300	36.496	116.472	90.830	33.335	-303.716	-174.607	29.354
1400	36.664	119.183	92.759	36.993	-303.217	-164.698	25.710
1500	36.801	121.717	94.606	40.667	-302.714	-154.820	22.557
1600	36.914	124.096	96.375	44.353	-302.211	-144.976	19.803
1700	37.008	126.337	98.073	48.049	-301.709	-135.162	17.376
1800	37.087	128.455	99.703	51.754	-301.212	-125.381	15.223
1900	37.155	130.462	101.269	55.466	-300.714	-115.625	13.300
2000	37.213	132.369	102.777	59.184	-300.226	-105.898	11.572

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 33.865 + 2.318\times10^{-3}T - 10.118\times10^{5}T^{-2}$

$H°- H°_{298} = 33.865\times10^{-3}T + 1.159\times10^{-6}T^{2} + 10.118\times10^{2}T^{-1} - 13.593$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr° = -310.608 + 4.169\times10^{-3}T + 0.477\times10^{-6}T^{2} + 676.150T^{-1}$

$\Delta Gr° = -310.608 - 4.169\times10^{-3}T\ln T - 0.477\times10^{-6}T^{2} + 338.075T^{-1} + 134.944\times10^{-3}T$

Source: Data from Chase (26).

$SSF_2(g)$

Thiothionyl Fluoride (ideal gas)

[Reaction: $S_2(g) + F_2(g) = SSF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15*	15.088	69.960	69.960	0	-126.610	-116.774	85.597
300	15.125	70.053	69.960	.028	-126.610	-116.713	85.024
400	16.702	74.640	70.575	1.626	-126.579	-113.417	61.967
500	17.655	78.478	71.782	3.348	-126.488	-110.135	48.139
600	18.252	81.753	73.178	5.145	-126.369	-106.876	38.929
700	18.643	84.598	74.611	6.991	-126.232	-103.638	32.357
800	18.911	87.106	76.019	8.870	-126.086	-100.420	27.433
900	19.101	89.345	77.377	10.771	-125.936	-97.221	23.608
1000	19.241	91.365	78.677	12.688	-125.786	-94.039	20.552
1100	19.346	93.204	79.915	14.618	-125.637	-90.870	18.054
1200	19.428	94.891	81.093	16.557	-125.491	-87.716	15.975
1300	19.491	96.449	82.216	18.503	-125.349	-84.575	14.218
1400	19.543	97.895	83.284	20.455	-125.214	-81.443	12.714
1500	19.584	99.245	84.304	22.411	-125.085	-78.323	11.411
1600	19.618	100.510	85.278	24.371	-124.962	-75.208	10.273
1700	19.647	101.700	86.209	26.334	-124.846	-72.102	9.269
1800	19.671	102.824	87.102	28.300	-124.736	-69.003	8.378
1900	19.691	103.888	87.957	30.268	-124.632	-65.909	7.581
2000	19.708	104.899	88.780	32.238	-124.536	-62.822	6.865

*Enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 18.814 + 0.634\times10^{-3}T - 3.480\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 18.814\times10^{-3}T + 0.317\times10^{-6}T^2 + 3.480\times10^{2}T^{-1} - 6.805$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr^\circ = -127.781 + 1.963\times10^{-3}T - 0.177\times10^{-6}T^2 + 179.200T^{-1}$

$\Delta Gr^\circ = -127.781 - 1.963\times10^{-3}T\ln T + 0.177\times10^{-6}T^2 + 89.600T^{-1} + 47.039\times10^{-3}T$

Source: Data from Chase (26) who estimated enthalpy of formation at 298 K.

$FS_2F(g)$

Difluorodisulfane (ideal gas)

[Reaction: $S_2(g) + F_2(g) = FS_2F(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15*	15.784	70.260	70.260	0	-111.110	-101.364	74.301
300	15.817	70.358	70.261	.029	-111.109	-101.303	73.798
400	17.202	75.116	70.901	1.686	-111.019	-98.047	53.570
500	18.020	79.050	72.148	3.451	-110.885	-94.818	41.444
600	18.525	82.383	73.583	5.280	-110.734	-91.619	33.372
700	18.853	85.265	75.051	7.150	-110.573	-88.446	27.614
800	19.077	87.798	76.489	9.047	-110.409	-85.296	23.302
900	19.236	90.055	77.874	10.963	-110.244	-82.168	19.953
1000	19.351	92.088	79.195	12.893	-110.081	-79.057	17.278
1100	19.439	93.936	80.451	14.833	-109.922	-75.961	15.092
1200	19.506	95.631	81.648	16.780	-109.768	-72.881	13.273
1300	19.559	97.194	82.784	18.733	-109.619	-69.813	11.736
1400	19.601	98.645	83.866	20.691	-109.478	-66.757	10.421
1500	19.635	99.999	84.897	22.653	-109.343	-63.712	9.283
1600	19.663	101.267	85.881	24.618	-109.215	-60.673	8.287
1700	19.687	102.460	86.821	26.586	-109.094	-57.642	7.410
1800	19.706	103.586	87.722	28.555	-108.981	-54.619	6.632
1900	19.723	104.651	88.584	30.527	-108.873	-51.599	5.935
2000	19.738	105.664	89.414	32.500	-108.774	-48.590	5.310

*Enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.051 + 0.494\times10^{-3}T - 3.035\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.051\times10^{-3}T + 0.247\times10^{-6}T^2 + 3.035\times10^{2}T^{-1} - 6.720$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr^\circ = -112.196 + 2.200\times10^{-3}T - 0.247\times10^{-6}T^2 + 134.700T^{-1}$

$\Delta Gr^\circ = -112.196 - 2.200\times10^{-3}T\ln T + 0.247\times10^{-6}T^2 + 67.350T^{-1} + 48.034\times10^{-3}T$

Source: Data from Chase (26) who estimated enthalpy of formation at 298 K.

$S_2F_{10}(g)$

Disulfur Decafluoride (ideal gas)

[Reaction: $S_2(g) + 5F_2(g) = S_2F_{10}(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	42.228	94.872	94.872	0	-524.110	-463.929	340.065
300	42.417	95.133	94.873	.078	-524.116	-463.556	337.696
400	50.530	108.535	96.645	4.756	-524.081	-443.357	242.236
500	55.625	120.400	100.234	10.083	-523.601	-423.223	184.988
600	58.900	130.851	104.484	15.820	-522.862	-403.216	146.869
700	61.072	140.105	108.925	21.826	-521.957	-383.344	119.684
800	62.564	148.363	113.348	28.012	-520.952	-363.613	99.333
900	63.605	155.795	117.658	34.323	-519.876	-344.005	83.535
1000	64.347	162.537	121.814	40.723	-518.763	-324.528	70.925
1100	64.861	168.695	125.800	47.184	-517.627	-305.157	60.628
1200	65.271	174.357	129.615	53.691	-516.477	-285.893	52.068
1300	65.553	179.593	133.260	60.233	-515.319	-266.721	44.839
1400	65.782	184.459	136.745	66.800	-514.169	-247.647	38.659
1500	65.943	189.004	140.079	73.387	-513.021	-228.651	33.314
1600	66.078	193.264	143.272	79.988	-511.881	-209.727	28.647
1700	66.160	197.272	146.331	86.600	-510.748	-190.873	24.538
1800	66.233	201.056	149.267	93.220	-509.632	-172.091	20.894
1900	66.296	204.639	152.088	99.846	-508.522	-153.366	17.641
2000	66.351	208.041	154.802	106.478	-507.432	-134.706	14.720

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 61.800 + 3.424\times10^{-3}T - 18.305\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 61.800\times10^{-3}T + 1.712\times10^{-6}T^2 + 18.305\times10^{2}T^{-1} - 24.717$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr^\circ = -531.636 + 10.917\times10^{-3}T + 0.522\times10^{-6}T^2 + 1259.700T^{-1}$

$\Delta Gr^\circ = -531.636 - 10.917\times10^{-3}T\ln T - 0.522\times10^{-6}T^2 + 629.850T^{-1} + 282.363\times10^{-3}T$

Source: Data from Chase (24).

$SbBr_3(g)$

Antimony Tribromide (ideal gas)

[Formation: $Sb(c,l) + 1.5Br_2(l,g) = SbBr_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	19.110	89.490	89.490	0	-46.500	-53.668	39.339
300	19.120	89.610	89.493	.035	-46.526	-53.712	39.128
332.6	19.224	91.588	89.603	.660	-46.980	-54.469	35.791
332.6	19.224	91.588	89.603	.660	-57.577	-54.469	35.791
400	19.440	95.160	90.248	1.965	-57.570	-53.844	29.419
500	19.590	99.520	91.686	3.917	-57.569	-52.915	23.129
600	19.670	103.100	93.298	5.881	-57.576	-51.987	18.936
700	19.730	106.130	94.914	7.851	-57.605	-51.046	15.937
800	19.760	108.770	96.489	9.825	-57.660	-50.112	13.690
900	19.780	111.100	97.987	11.802	-57.751	-49.164	11.939
903.9	19.781	111.186	98.043	11.879	-57.755	-49.127	11.878
903.9	19.781	111.186	98.043	11.879	-62.505	-49.127	11.878
1000	19.800	113.180	99.398	13.782	-62.620	-47.697	10.424

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
903.9 K, melting point of Sb; ΔH° = 4.750 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 19.827 + 0.042\times10^{-3}T - 0.648\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.827\times10^{-3}T + 0.021\times10^{-6}T^2 + 0.648\times10^{2}T^{-1} - 6.131$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -43.004 - 12.398\times10^{-3}T - 1.001\times10^{-6}T^2 + 86.400T^{-1}$

$\Delta Gf^\circ = -43.004 + 12.398\times10^{-3}T\ln T + 1.001\times10^{-6}T^2 + 43.200T^{-1} - 107.186\times10^{-3}T$

332.6-903.9 K: $\Delta Hf^\circ = -58.005 + 1.344\times10^{-3}T - 1.234\times10^{-6}T^2 + 39.300T^{-1}$

$\Delta Gf^\circ = -58.005 - 1.344\times10^{-3}T\ln T + 1.234\times10^{-6}T^2 + 19.650T^{-1} + 17.847\times10^{-3}T$

903.9-1000 K: $\Delta Hf^\circ = -61.509 - 1.068\times10^{-3}T - 0.062\times10^{-6}T^2 + 17.700T^{-1}$

$\Delta Gf^\circ = -61.509 + 1.068\times10^{-3}T\ln T + 0.062\times10^{-6}T^2 + 8.850T^{-1} + 6.377\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Other data from Clark (32).

$SbCl_3(g)$

Antimony Trichloride (ideal gas)

[Formation: $Sb(c,1) + 1.5Cl_2(g) = SbCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	18.340	81.020	81.020	0	-75.000	-72.080	52.835
300	18.350	81.130	81.020	.034	-75.000	-72.060	52.495
400	18.970	86.500	81.740	1.904	-74.987	-71.080	38.836
500	19.280	90.770	83.134	3.818	-74.979	-70.102	30.641
600	19.450	94.310	84.718	5.755	-74.986	-69.136	25.182
700	19.560	97.310	86.301	7.706	-75.010	-68.151	21.277
800	19.630	99.930	87.848	9.666	-75.065	-67.176	18.351
900	19.680	102.250	89.326	11.632	-75.155	-66.186	16.072
903.9	19.682	102.335	89.382	11.709	-75.159	-66.146	15.993
903.9	19.682	102.335	89.382	11.709	-79.909	-66.146	15.993
1000	19.720	104.320	90.718	13.602	-80.024	-64.677	14.135

Phase change: 903.9 K, melting point of Sb; $\Delta H^\circ = 4.750$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 19.688 + 0.168\times10^{-3}T - 1.243\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.688\times10^{-3}T + 0.084\times10^{-6}T^2 + 1.243\times10^{2}T^{-1} - 6.294$

Formation equations (kcal/mol):

298.15-903.9 K: $\Delta Hf^\circ = -75.443 + 1.360\times10^{-3}T - 1.220\times10^{-6}T^2 + 43.450T^{-1}$

$\Delta Gf^\circ = -75.443 - 1.360\times10^{-3}T\ln T + 1.220\times10^{-6}T^2 + 21.725T^{-1} + 18.417\times10^{-3}T$

903.9-1000 K: $\Delta Hf^\circ = -78.946 - 1.053\times10^{-3}T - 0.048\times10^{-6}T^2 + 21.850T^{-1}$

$\Delta Gf^\circ = -78.946 + 1.053\times10^{-3}T\ln T + 0.048\times10^{-6}T^2 + 10.925T^{-1} + 6.948\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Other data from Clark (32).

SbF_3(c,l,g)
Antimony Trifluoride
[Formation: $Sb(c,l) + 1.5F_2(g) = SbF_3(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	21.563	30.410	30.410	0	-218.800	-202.958	148.770
300	21.602	30.544	30.411	.040	-218.792	-202.859	147.781
400	23.683	37.043	31.283	2.304	-218.294	-197.619	107.972
500	25.765	42.551	32.997	4.777	-217.654	-192.519	84.149
560	27.014	45.541	34.184	6.360	-217.196	-189.534	73.968
560	35.200	55.255	34.184	11.800	-211.756	-189.534	73.968
600	35.200	57.684	35.671	13.208	-211.108	-187.969	68.467
619	35.200	58.781	36.363	13.877	-210.802	-187.241	66.108
619	18.843	85.416	36.363	30.364	-194.315	-187.241	66.108
700	19.065	87.747	42.176	31.900	-194.347	-186.310	58.168
800	19.249	90.306	48.036	33.816	-194.410	-185.164	50.584
900	19.369	92.581	52.861	35.748	-194.504	-183.999	44.680
903.9	19.372	92.665	53.033	35.824	-194.509	-183.953	44.477
903.9	19.372	92.665	53.033	35.824	-199.259	-183.953	44.477
1000	19.439	94.626	56.937	37.689	-199.382	-182.326	39.847

*Heat capacity at 298 K and data for gas estimated.

Phase changes: 560 K, melting point of SbF_3; $\Delta H°$ = 5.440 kcal/mol.
619 K, boiling point of SbF_3; $\Delta H°$ = 16.487 kcal/mol.
903.9 K, melting point of Sb; $\Delta H°$ = 4.750 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-560 K: $Cp° = 15.357 + 20.818\times10^{-3}T$
$H°- H°_{298} = 15.357\times10^{-3}T + 10.409\times10^{-6}T^2 - 5.504$
560-619 K: $Cp° = 35.200$
$H°- H°_{298} = 35.200\times10^{-3}T - 7.912$
619-1000 K: $Cp° = 19.924 - 0.068\times10^{-3}T - 3.980\times10^{5}T^{-2}$
$H°- H°_{298} = 19.924\times10^{-3}T - 0.034\times10^{-6}T^2 + 3.980\times10^{2}T^{-1} + 17.401$

Formation equations (kcal/mol):

298.15-560 K: $\Delta Hf° = -218.421 - 2.493\times10^{-3}T + 8.976\times10^{-6}T^2 - 129.150T^{-1}$
$\Delta Gf° = -218.421 + 2.493\times10^{-3}T\ln T - 8.976\times10^{-6}T^2 - 64.575T^{-1} + 41.063\times10^{-3}T$
560-619 K: $\Delta Hf° = -220.829 + 17.350\times10^{-3}T - 1.433\times10^{-6}T^2 - 129.150T^{-1}$
$\Delta Gf° = -220.829 - 17.350\times10^{-3}T\ln T + 1.433\times10^{-6}T^2 - 64.575T^{-1} + 165.099\times10^{-3}T$
619-903.9 K: $\Delta Hf° = -195.516 + 2.074\times10^{-3}T - 1.467\times10^{-6}T^2 + 268.850T^{-1}$
$\Delta Gf° = -195.516 - 2.074\times10^{-3}T\ln T + 1.467\times10^{-6}T^2 + 134.425T^{-1} + 25.470\times10^{-3}T$
903.9-1000 K: $\Delta Hf° = -199.020 - 0.338\times10^{-3}T - 0.295\times10^{-6}T^2 + 247.250T^{-1}$
$\Delta Gf° = -199.020 + 0.338\times10^{-3}T\ln T + 0.295\times10^{-6}T^2 + 123.625T^{-1} + 14.001\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Data for crystal and liquid based on Cubicciotti (45). Gas data based on those estimated by Cubicciotti (45).

$SbF_3(g)$

Antimony Trifluoride (ideal gas)

[Formation: $Sb(c,l) + 1.5F_2(g) = SbF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	16.313	72.400	72.400	0	-194.200	-190.877	139.915
300	16.349	72.501	72.401	.030	-194.202	-190.856	139.037
400	17.685	77.412	73.062	1.740	-194.257	-189.730	103.662
500	18.374	81.439	74.347	3.546	-194.284	-188.594	82.433
600	18.791	84.829	75.819	5.406	-194.309	-187.458	68.281
700	19.065	87.747	77.318	7.300	-194.346	-186.310	58.168
800	19.249	90.306	78.786	9.216	-194.410	-185.164	50.584
900	19.369	92.581	80.194	11.148	-194.504	-183.999	44.680
903.9	19.372	92.665	80.248	11.224	-194.509	-183.953	44.477
903.9	19.372	92.665	80.248	11.224	-199.259	-183.953	44.477
1000	19.439	94.626	81.537	13.089	-199.382	-182.325	39.847

*Data except enthalpy of formation at 298 K estimated.

Phase change: 903.9 K, melting point of Sb; $\Delta H° = 4.750$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 19.105 + 0.674\times10^{-3}T - 2.660\times10^{5}T^{-2}$

$H°- H°_{298} = 19.105\times10^{-3}T + 0.337\times10^{-6}T^2 + 2.660\times10^{2}T^{-1} - 6.618$

Formation equations (kcal/mol):

298.15-903.9 K: $\Delta Hf° = -194.936 + 1.255\times10^{-3}T - 1.096\times10^{-6}T^2 + 136.850T^{-1}$

$\Delta Gf° = -194.936 - 1.255\times10^{-3}T\ln T + 1.096\times10^{-6}T^2 + 68.425T^{-1} + 19.666\times10^{-3}T$

903.9-1000 K: $\Delta Hf° = -198.439 - 1.157\times10^{-3}T + 0.076\times10^{-6}T^2 + 115.250T^{-1}$

$\Delta Gf° = -198.439 + 1.157\times10^{-3}T\ln T - 0.076\times10^{-6}T^2 + 57.625T^{-1} + 8.197\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Cubicciotti (45). Other data based on those estimated by Cubicciotti (45).

SbI_3(c,l,g)
Antimony Triiodide
[Formation: $Sb(c,l) + 1.5I_2(c,l,g) = SbI_3(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	23.440	52.320	52.320	0	-24.000	-23.941	17.549
300	23.500	52.465	52.332	.040	-24.007	-23.943	17.442
386.8	25.149	58.642	53.067	2.156	-24.233	-23.893	13.500
386.8	25.149	58.642	53.067	2.156	-29.796	-23.893	13.500
400	25.400	59.490	53.265	2.490	-29.927	-23.690	12.943
444	26.400	62.193	54.017	3.630	-30.332	-22.979	11.311
444	34.400	74.468	54.017	9.080	-24.882	-22.979	11.311
458.4	34.400	75.566	54.677	9.575	-24.894	-22.916	10.925
458.4	34.400	75.566	54.677	9.575	-39.925	-22.916	10.925
500	34.400	78.554	56.534	11.010	-39.311	-21.393	9.351
600	34.400	84.826	60.743	14.450	-37.856	-17.952	6.539
667	34.400	88.469	63.349	16.755	-36.893	-15.779	5.170
667	19.803	112.634	63.349	32.873	-20.775	-15.779	5.170
700	19.810	113.590	65.694	33.527	-20.787	-15.530	4.849
800	19.820	116.240	71.854	35.509	-20.842	-14.782	4.038
900	19.830	118.570	76.912	37.492	-20.936	-14.013	3.403
903.9	19.830	118.656	77.092	37.569	-20.940	-13.983	3.381
903.9	19.830	118.656	77.092	37.569	-25.690	-13.983	3.381
1000	19.840	120.660	81.184	39.476	-25.808	-12.736	2.783

*Heat capacity at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
444 K, melting point of SbI_3; $\Delta H°$ = 5.450 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
667 K, boiling point of SbI_3; $\Delta H°$ = 16.118 kcal/mol.
903.9 K, melting point of Sb; $\Delta H°$ = 4.750 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-444 K: $Cp° = 17.159 + 20.554\times10^{-3}T + 0.136\times10^{5}T^{-2}$
$H°- H°_{298} = 17.159\times10^{-3}T + 10.277\times10^{-6}T^{2} - 0.136\times10^{2}T^{-1} - 5.984$

444-667 K: $Cp° = 34.415$
$H°- H°_{298} = 34.415\times10^{-3}T - 6.200$

667-1000 K: $Cp° = 19.966 - 0.074\times10^{-3}T - 0.509\times10^{5}T^{-2}$
$H°- H°_{298} = 19.966\times10^{-3}T - 0.037\times10^{-6}T^{2} + 0.509\times10^{2}T^{-1} + 19.496$

SbI_3(c,l,g) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -22.477 - 7.244\times10^{-3}T + 6.867\times10^{-6}T^2 + 8.000T^{-1}$

$\Delta Gf^\circ = -22.477 + 7.244\times10^{-3}T\ln T - 6.867\times10^{-6}T^2 + 4.000T^{-1} - 44.184\times10^{-3}T$

386.8-444 K: $\Delta Hf^\circ = -24.660 - 16.851\times10^{-3}T + 9.105\times10^{-6}T^2 + 8.000T^{-1}$

$\Delta Gf^\circ = -24.660 + 16.851\times10^{-3}T\ln T - 9.105\times10^{-6}T^2 + 4.000T^{-1} - 94.907\times10^{-3}T$

444-458.4 K: $\Delta Hf^\circ = -24.876 + 0.405\times10^{-3}T - 1.172\times10^{-6}T^2 + 21.600T^{-1}$

$\Delta Gf^\circ = -24.876 - 0.405\times10^{-3}T\ln T + 1.172\times10^{-6}T^2 + 10.800T^{-1} + 6.172\times10^{-3}T$

458.4-667 K: $\Delta Hf^\circ = -46.946 + 15.915\times10^{-3}T - 1.274\times10^{-6}T^2 - 1.350T^{-1}$

$\Delta Gf^\circ = -46.946 - 15.915\times10^{-3}T\ln T + 1.274\times10^{-6}T^2 - 0.675T^{-1} + 149.367\times10^{-3}T$

667-903.9 K: $\Delta Hf^\circ = -21.251 + 1.466\times10^{-3}T - 1.311\times10^{-6}T^2 + 49.550T^{-1}$

$\Delta Gf^\circ = -21.251 - 1.466\times10^{-3}T\ln T + 1.311\times10^{-6}T^2 + 24.775T^{-1} + 16.802\times10^{-3}T$

903.9-1000 K: $\Delta Hf^\circ = -24.754 - 0.946\times10^{-3}T - 0.139\times10^{-6}T^2 + 27.950T^{-1}$

$\Delta Gf^\circ = -24.754 + 0.946\times10^{-3}T\ln T + 0.139\times10^{-6}T^2 + 13.975T^{-1} + 5.333\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Entropy at 298 K based on Ferro (79). Heat capacity at 298 K estimated. Data for crystal and liquid based on Cubicciotti (48). Data for gas from Clark (32).

$SbI_3(g)$

Antimony Triiodide (ideal gas)

[Formation: $Sb(c,l) + 1.5I_2(c,l,g) = SbI_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	19.540	96.770	96.770	0	1.600	-11.594	8.499
300	19.540	96.890	96.770	.036	1.589	-11.674	8.505
386.8	19.662	101.880	97.386	1.738	.949	-15.436	8.721
386.8	19.662	101.880	97.386	1.738	-4.614	-15.436	8.721
400	19.680	102.540	97.545	1.998	-4.819	-15.802	8.634
458.4	19.721	105.226	98.356	3.149	-5.720	-17.338	8.266
458.4	19.721	105.226	98.356	3.149	-20.752	-17.338	8.266
500	19.750	106.940	99.000	3.970	-20.751	-17.026	7.442
600	19.790	110.540	100.628	5.947	-20.760	-16.283	5.931
700	19.810	113.590	102.266	7.927	-20.787	-15.530	4.849
800	19.820	116.240	103.854	9.909	-20.842	-14.782	4.038
900	19.830	118.570	105.357	11.892	-20.936	-14.013	3.403
903.9	19.830	118.656	105.414	11.969	-20.940	-13.983	3.381
903.9	19.830	118.656	105.414	11.969	-25.690	-13.983	3.381
1000	19.840	120.660	106.784	13.876	-25.808	-12.736	2.783

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
903.9 K, melting point of Sb; $\Delta H°$ = 4.750 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 19.847 + 0.028\times10^{-3}T - 0.280\times10^{5}T^{-2}$

$H°-H°_{298} = 19.847\times10^{-3}T + 0.014\times10^{-6}T^2 + 0.280\times10^{2}T^{-1} - 6.013$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = 3.094 - 4.556\times10^{-3}T - 3.396\times10^{-6}T^2 + 49.600T^{-1}$

$\Delta Gf° = 3.094 + 4.556\times10^{-3}T\ln T + 3.396\times10^{-6}T^2 + 24.800T^{-1} - 76.517\times10^{-3}T$

386.8-458.4 K: $\Delta Hf° = 0.911 - 14.163\times10^{-3}T - 1.158\times10^{-6}T^2 + 49.600T^{-1}$

$\Delta Gf° = 0.911 + 14.163\times10^{-3}T\ln T + 1.158\times10^{-6}T^2 + 24.800T^{-1} - 127.240\times10^{-3}T$

458.4-903.9 K: $\Delta Hf° = -21.158 + 1.348\times10^{-3}T - 1.260\times10^{-6}T^2 + 26.650T^{-1}$

$\Delta Gf° = -21.158 - 1.348\times10^{-3}T\ln T + 1.260\times10^{-6}T^2 + 13.325T^{-1} + 15.955\times10^{-3}T$

903.9-1000 K: $\Delta Hf° = -24.662 - 1.064\times10^{-3}T - 0.088\times10^{-6}T^2 + 5.050T^{-1}$

$\Delta Gf° = -24.662 + 1.064\times10^{-3}T\ln T + 0.088\times10^{-6}T^2 + 2.525T^{-1} + 4.486\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Ferro (79). Other data from Clark (32).

$ScCl_3(c,l)$
Scandium Trichloride
[Formation: $Sc(c) + 1.5Cl_2(g) = ScCl_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	21.900	30.400	30.400	0	-221.100	-203.862	149.433
300	21.939	30.536	30.400	.041	-221.092	-203.754	148.433
400	23.374	37.071	31.281	2.316	-220.684	-198.037	108.201
500	24.057	42.369	32.987	4.691	-220.223	-192.426	84.108
600	24.431	46.790	34.928	7.117	-219.749	-186.912	68.082
700	24.746	50.580	36.901	9.575	-219.275	-181.475	56.658
800	25.191	53.911	38.822	12.071	-218.793	-176.104	48.109
900	25.934	56.917	40.668	14.624	-218.283	-170.809	41.478
1000	27.131	59.707	42.435	17.272	-217.708	-165.568	36.185
1100	28.936	62.372	44.127	20.070	-217.016	-160.380	31.864
1200	31.501	64.993	45.755	23.085	-216.141	-155.240	28.273
1240	32.773	66.046	46.393	24.370	-215.722	-153.216	27.004
1240	34.300	78.522	46.393	39.840	-200.252	-153.216	27.004
1300	34.300	80.143	47.914	41.898	-199.503	-150.982	25.382
1400	34.300	82.685	50.308	45.328	-198.287	-147.303	22.995

*Entropy and heat capacity at 298 K estimated.

Phase change: 1240 K, melting point of $ScCl_3$; ΔH° = 15.470 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1240 K: $Cp^\circ = 19.618 + 8.184\times10^{-3}T - 0.142\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.618\times10^{-3}T + 4.092\times10^{-6}T^2 + 0.142\times10^{2}T^{-1} - 6.260$

1240-1400 K: $Cp^\circ = 34.300$

$H^\circ - H^\circ_{298} = 34.300\times10^{-3}T - 2.692$

Formation equations (kcal/mol):

298.15-1240 K: $\Delta Hf^\circ = -221.607 + 1.494\times10^{-3}T + 2.621\times10^{-6}T^2 - 51.150T^{-1}$

$\Delta Gf^\circ = -221.607 - 1.494\times10^{-3}T\ln T - 2.621\times10^{-6}T^2 - 25.575T^{-1} + 69.093\times10^{-3}T$

1240-1400 K: $\Delta Hf^\circ = -218.039 + 16.175\times10^{-3}T - 1.471\times10^{-6}T^2 - 65.350T^{-1}$

$\Delta Gf^\circ = -218.039 - 16.175\times10^{-3}T\ln T + 1.471\times10^{-6}T^2 - 32.675T^{-1} + 165.724\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (254). Entropy and heat capacity at 298 K estimated. High-temperature data based on Dworkin (69).

$ScF_3(c,l)$
Scandium Trifluoride
[Formation: $Sc(c,l) + 1.5F_2(g) = ScF_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	20.000	23.400	23.400	0	-385.200	-368.043	269.779
300	20.050	23.520	23.400	.037	-385.195	-367.935	268.037
400	21.740	29.560	24.205	2.142	-384.865	-362.229	197.910
500	22.580	34.510	25.784	4.363	-384.484	-356.610	155.872
600	23.080	38.670	27.592	6.647	-384.095	-351.072	127.876
700	23.400	42.260	29.441	8.973	-383.707	-345.600	107.900
800	23.650	45.400	31.243	11.326	-383.332	-340.177	92.931
900	23.830	48.200	32.978	13.700	-382.972	-334.819	81.304
1000	23.990	50.720	34.628	16.092	-382.633	-329.490	72.009
1100	24.130	53.010	36.194	18.498	-382.316	-324.181	64.408
1200	24.250	55.110	37.679	20.917	-382.024	-318.877	58.075
1300	24.360	57.060	39.100	23.348	-381.757	-313.653	52.729
1400	24.470	58.870	40.449	25.790	-381.523	-308.433	48.148
1500	24.570	60.560	41.733	28.241	-381.321	-303.213	44.178
1600	24.660	62.150	42.961	30.703	-381.152	-298.017	40.707
1608	24.668	62.273	43.056	30.900	-381.139	-297.594	40.447
1608	24.668	62.273	43.056	30.900	-382.097	-297.594	40.447
1700	24.760	63.650	44.136	33.174	-382.048	-292.772	37.638
1800	24.840	65.060	45.252	35.654	-381.994	-287.517	34.909
1812	24.869	65.225	45.384	35.952	-381.987	-286.887	34.602
1812	24.869	65.225	45.384	35.952	-385.356	-286.887	34.602
1825	24.900	65.410	45.532	36.275	-385.348	-286.191	34.272
1825	21.240	73.610	45.532	51.244	-370.379	-286.191	34.272
1900	21.240	74.460	46.651	52.837	-370.606	-282.716	32.519
2000	21.240	75.540	48.060	54.961	-370.915	-278.069	30.386

*Heat capacity at 298 K estimated.

Phase changes: 1608 K, α - β transition point of Sc; $\Delta H°$ = 0.958 kcal/mol.
1812 K, melting point of Sc; $\Delta H°$ = 3.369 kcal/mol.
1825 K, melting point of ScF_3; $\Delta H°$ = 14.969 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1825 K: $Cp° = 23.552 + 0.776\times10^{-3}T - 3.363\times10^{5}T^{-2}$

$H°- H°_{298} = 23.552\times10^{-3}T + 0.388\times10^{-6}T^{2} + 3.363\times10^{2}T^{-1} - 8.184$

1825-2000 K: $Cp° = 21.240$

$H°- H°_{298} = 21.240\times10^{-3}T + 12.481$

ScF_3(c,l) - Continued

Formation equations (kcal/mol):

298.15-1608 K: $\Delta Hf^\circ = -387.600 + 5.906\times10^{-3}T - 1.212\times10^{-6}T^2 + 222.650T^{-1}$

$\Delta Gf^\circ = -387.600 - 5.906\times10^{-3}T\ln T + 1.212\times10^{-6}T^2 + 111.325T^{-1} + 97.630\times10^{-3}T$

1608-1812 K: $\Delta Hf^\circ = -382.854 + 0.220\times10^{-3}T + 0.127\times10^{-6}T^2 + 185.550T^{-1}$

$\Delta Gf^\circ = -382.854 - 0.220\times10^{-3}T\ln T - 0.127\times10^{-6}T^2 + 92.775T^{-1} + 54.861\times10^{-3}T$

1812-1825 K: $\Delta Hf^\circ = -386.223 + 0.220\times10^{-3}T + 0.127\times10^{-6}T^2 + 185.550T^{-1}$

$\Delta Gf^\circ = -386.223 - 0.220\times10^{-3}T\ln T - 0.127\times10^{-6}T^2 + 92.775T^{-1} + 56.720\times10^{-3}T$

1825-2000 K: $\Delta Hf^\circ = -365.558 - 2.092\times10^{-3}T - 0.261\times10^{-6}T^2 - 150.750T^{-1}$

$\Delta Gf^\circ = -365.558 + 2.092\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 - 75.375T^{-1} + 27.377\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Rinehart (199. Heat capacity at 298 K estimated. High-temperature data based on Spedding (222).

$ScF_3(g)$

Scandium Trifluoride (ideal gas)

[Formation: $Sc(c) + 1.5F_2(g) = ScF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	16.190	72.770	72.770	0	-295.300	-292.863	214.671
300	16.220	72.870	72.770	.030	-295.302	-292.847	213.336
400	17.400	77.720	73.420	1.720	-295.386	-292.014	159.547
500	18.140	81.680	74.680	3.500	-295.447	-291.158	127.263
600	18.600	85.040	76.157	5.330	-295.512	-290.311	105.744
700	18.910	87.930	77.630	7.210	-295.569	-289.432	90.364
800	19.120	90.470	79.083	9.110	-295.647	-288.549	78.827
900	19.270	92.730	80.474	11.030	-295.742	-287.666	69.854
1000	19.380	94.760	81.790	12.970	-295.855	-286.752	62.669
1100	19.460	96.610	83.055	14.910	-296.004	-285.829	56.788
1200	19.520	98.310	84.260	16.860	-296.181	-284.874	51.882
1300	19.570	99.880	85.411	18.810	-296.395	-283.957	47.737
1400	19.610	101.330	86.494	20.770	-296.643	-282.997	44.177
1500	19.640	102.680	87.527	22.730	-296.931	-282.004	41.087
1600	19.670	103.950	88.512	24.700	-297.254	-281.000	38.382
1608	19.672	104.048	88.590	24.857	-297.282	-280.912	38.179
1608	19.672	104.048	88.590	24.857	-298.240	-280.912	38.179
1700	19.690	105.140	89.452	26.670	-298.652	-279.909	35.984
1800	19.710	106.270	90.359	28.640	-299.108	-278.809	33.852

Phase change: 1608 K, transition point of Sc; $\Delta H° = 0.958$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1800 K: $Cp° = 18.932 + 0.606\times10^{-3}T - 2.598\times10^{5}T^{-2}$

$H°- H°_{298} = 18.932\times10^{-3}T + 0.303\times10^{-6}T^{2} + 2.598\times10^{2}T^{-1} - 6.543$

Formation equations (kcal/mol):

298.15-1608 K: $\Delta Hf° = -296.058 + 1.286\times10^{-3}T - 1.297\times10^{-6}T^{2} + 146.150T^{-1}$

$\Delta Gf° = -296.058 - 1.286\times10^{-3}T\ln T + 1.297\times10^{-6}T^{2} + 73.075T^{-1} + 16.836\times10^{-3}T$

1608-1800 K: $\Delta Hf° = -291.312 - 4.400\times10^{-3}T + 0.042\times10^{-6}T^{2} + 109.050T^{-1}$

$\Delta Gf° = -291.312 + 4.400\times10^{-3}T\ln T - 0.042\times10^{-6}T^{2} + 54.525T^{-1} - 25.933\times10^{-3}T$

Source: Data from Rinehart (199).

$SeBr_2(g)$

Selenium Dibromide (ideal gas)

[Reaction: $0.5Se_2(g) + Br_2(l,g) = SeBr_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15*	13.240	75.760	75.760	0	-21.650	-24.715	18.117
300	13.250	75.842	75.760	.025	-21.667	-24.733	18.018
332.6	13.341	77.214	75.835	.458	-21.982	-25.050	16.460
332.6	13.341	77.214	75.835	.458	-29.047	-25.050	16.460
400	13.530	79.710	76.292	1.367	-29.064	-24.246	13.247
500	13.660	82.740	77.284	2.728	-29.089	-23.035	10.068
600	13.740	85.240	78.410	4.098	-29.113	-21.824	7.949
700	13.780	87.360	79.540	5.474	-29.135	-20.605	6.433
800	13.810	89.200	80.632	6.854	-29.154	-19.381	5.295
900	13.830	90.830	81.679	8.236	-29.173	-18.162	4.410
1000	13.840	92.290	82.671	9.619	-29.190	-16.943	3.703
1100	13.850	93.610	83.606	11.004	-29.204	-15.715	3.122
1200	13.860	94.810	84.485	12.390	-29.215	-14.481	2.637
1300	13.870	95.920	85.322	13.777	-29.224	-13.251	2.228
1400	13.880	96.950	86.119	15.164	-29.232	-12.027	1.877
1500	13.880	97.910	86.875	16.552	-29.237	-10.802	1.574
1600	13.880	98.810	87.597	17.940	-29.240	-9.581	1.309
1700	13.890	99.650	88.280	19.329	-29.241	-8.343	1.073
1800	13.890	100.440	88.930	20.718	-29.240	-7.110	.863
1900	13.890	101.190	89.555	22.107	-29.236	-5.879	.676
2000	13.900	101.900	90.152	23.497	-29.230	-4.648	.508

*Data except enthalpy of formation at 298 K estimated.

Phase change: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.904 - 0.590\times10^{5}T^{-2}$

$H°- H°_{298} = 13.904\times10^{-3}T + 0.590\times10^{2}T^{-1} - 4.343$

Reaction equations (kcal/mol):

298.15-332.6 K: $\Delta Hr° = -18.932 - 9.519\times10^{-3}T + 0.260\times10^{-6}T^{2} + 29.050T^{-1}$

$\Delta Gr° = -18.932 + 9.519\times10^{-3}T\ln T - 0.260\times10^{-6}T^{2} + 14.525T^{-1} - 73.717\times10^{-3}T$

332.6-2000 K: $\Delta Hr° = -28.933 - 0.358\times10^{-3}T + 0.105\times10^{-6}T^{2} - 2.350T^{-1}$

$\Delta Gr° = -28.933 + 0.358\times10^{-3}T\ln T - 0.105\times10^{-6}T^{2} - 1.175T^{-1} + 9.638\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Other data are those estimated by Mills (159).

$Se_2Br_2(g)$

Diselenium Dibromide (ideal gas)

[Reaction: $Se_2(g) + Br_2(l,g) = Se_2Br_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	19.040	90.350	90.350	0	-26.300	-25.039	18.354
300	19.050	90.462	90.352	.033	-26.318	-25.031	18.235
332.6	19.177	92.434	90.461	.656	-26.604	-24.877	16.346
332.6	19.177	92.434	90.461	.656	-33.669	-24.877	16.346
400	19.440	96.020	91.110	1.964	-33.624	-23.105	12.624
500	19.640	100.380	92.542	3.919	-33.559	-20.482	8.953
600	19.770	103.970	94.153	5.890	-33.487	-17.873	6.510
700	19.860	107.030	95.784	7.872	-33.408	-15.278	4.770
800	19.940	109.680	97.353	9.862	-33.321	-12.684	3.465
900	20.010	112.040	98.862	11.860	-33.226	-10.119	2.457
1000	20.070	114.150	100.286	13.864	-33.121	-7.559	1.652

Phase change: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 19.752 + 0.382\times10^{-3}T - 0.734\times10^{5}T^{-2}$

$H°- H°_{298} = 19.752\times10^{-3}T + 0.191\times10^{-6}T^2 + 0.734\times10^{2}T^{-1} - 6.152$

Reaction equations (kcal/mol):

298.15-332.6 K: $\Delta Hr° = -23.715 - 9.003\times10^{-3}T + 0.610\times10^{-6}T^2 + 13.500T^{-1}$

$\Delta Gr° = -23.715 + 9.003\times10^{-3}T\ln T - 0.610\times10^{-6}T^2 + 6.750T^{-1} - 55.630\times10^{-3}T$

332.6-1000 K: $\Delta Hr° = -33.716 + 0.158\times10^{-3}T + 0.455\times10^{-6}T^2 - 17.900T^{-1}$

$\Delta Gr° = -33.716 - 0.158\times10^{-3}T\ln T - 0.455\times10^{-6}T^2 - 8.950T^{-1} + 27.725\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Other data from Mills (159).

$SeCl_2(g)$

Selenium Dichloride (ideal gas)

[Reaction: $0.5Se_2(g) + Cl_2(g) = SeCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	12.800	70.650	70.650	0	-24.650	-21.150	15.503
300	12.810	70.730	70.650	.024	-24.650	-21.128	15.392
400	13.270	74.490	71.158	1.333	-24.668	-19.950	10.900
500	13.490	77.480	72.136	2.672	-24.687	-18.770	8.204
600	13.610	79.950	73.238	4.027	-24.706	-17.585	6.405
700	13.680	82.060	74.357	5.392	-24.724	-16.400	5.120
800	13.730	83.890	75.438	6.762	-24.744	-15.210	4.155
900	13.760	85.500	76.459	8.137	-24.761	-14.009	3.402
1000	13.790	86.960	77.446	9.514	-24.778	-12.824	2.803
1100	13.810	88.270	78.366	10.894	-24.792	-11.621	2.309
1200	13.820	89.470	79.240	12.276	-24.804	-10.420	1.898
1300	13.840	90.580	80.073	13.659	-24.814	-9.223	1.551
1400	13.850	91.610	80.865	15.043	-24.823	-8.032	1.254
1500	13.860	92.560	81.608	16.428	-24.829	-6.825	.994
1600	13.860	93.460	82.326	17.814	-24.833	-5.635	.770
1700	13.870	94.300	83.005	19.201	-24.835	-4.425	.569
1800	13.880	95.090	83.652	20.588	-24.836	-3.225	.392
1900	13.880	95.840	84.274	21.976	-24.833	-2.023	.233
2000	13.890	96.550	84.868	23.365	-24.829	-.821	.090

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.856 + 0.028\times10^{-3}T - 0.946\times10^{5}T^{-2}$

$H°- H°_{298} = 13.856\times10^{-3}T + 0.014\times10^{-6}T^{2} + 0.946\times10^{2}T^{-1} - 4.450$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr° = -24.555 - 0.303\times10^{-3}T + 0.086\times10^{-6}T^{2} - 3.650T^{-1}$

$\Delta Gr° = -24.555 + 0.303\times10^{-3}T\ln T - 0.086\times10^{-6}T^{2} - 1.825T^{-1} + 9.741\times10^{-3}T$

Source: Data from Mills (159).

$Se_2Cl_2(g)$

Diselenium Dichloride (ideal gas)

[Reaction: $Se_2(g) + Cl_2(g) = Se_2Cl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	18.580	84.560	84.560	0	-38.500	-30.471	22.335
300	18.690	84.680	84.563	.035	-38.498	-30.422	22.162
400	19.160	90.120	85.300	1.928	-38.430	-27.740	15.156
500	19.440	94.430	86.710	3.860	-38.359	-25.075	10.960
600	19.610	97.990	88.302	5.813	-38.286	-22.426	8.169
700	19.730	101.020	89.906	7.780	-38.207	-19.786	6.177
800	19.810	103.660	91.464	9.757	-38.124	-17.158	4.687
900	19.890	106.000	92.953	11.742	-38.033	-14.546	3.532
1000	19.950	108.100	94.366	13.734	-37.934	-11.946	2.611

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 19.746 + 0.304\times10^{-3}T - 1.117\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.746\times10^{-3}T + 0.152\times10^{-6}T^2 + 1.117\times10^{2}T^{-1} - 6.275$

Reaction equations (kcal/mol):

298.15-1000 K: $\Delta Hr^\circ = -38.555 + 0.255\times10^{-3}T + 0.383\times10^{-6}T^2 - 16.500T^{-1}$

$\Delta Gr^\circ = -38.555 - 0.255\times10^{-3}T\ln T - 0.383\times10^{-6}T^2 - 8.250T^{-1} + 28.773\times10^{-3}T$

Source: Data from Mills (159).

SeF(g)

Selenium Monofluoride (ideal gas)

[Reaction: $0.5Se_2(g) + 0.5F_2(g) = SeF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15*	7.710	55.780	55.780	0	-26.650	-27.383	20.072
300	7.720	55.830	55.783	.014	-26.652	-27.389	19.952
400	8.180	58.120	56.087	.813	-26.735	-27.619	15.090
500	8.400	59.980	56.694	1.643	-26.811	-27.835	12.167
600	8.520	61.520	57.370	2.490	-26.885	-28.032	10.211
700	8.600	62.840	58.059	3.347	-26.956	-28.216	8.809
800	8.660	63.990	58.728	4.210	-27.028	-28.388	7.755
900	8.700	65.020	59.378	5.078	-27.098	-28.561	6.935
1000	8.740	65.930	59.980	5.950	-27.166	-28.713	6.275
1100	8.770	66.770	60.565	6.825	-27.231	-28.869	5.736
1200	8.790	67.530	61.111	7.703	-27.292	-29.011	5.284
1300	8.810	68.240	61.638	8.583	-27.351	-29.157	4.902
1400	8.830	68.890	62.129	9.466	-27.406	-29.291	4.572
1500	8.850	69.500	62.600	10.350	-27.459	-29.424	4.287
1600	8.870	70.070	63.048	11.236	-27.509	-29.552	4.037
1700	8.880	70.610	63.479	12.123	-27.556	-29.675	3.815
1800	8.900	71.120	63.891	13.012	-27.599	-29.806	3.619
1900	8.920	71.600	64.283	13.903	-27.638	-29.926	3.442
2000	8.930	72.060	64.662	14.795	-27.675	-30.052	3.284

*Data estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.705 + 0.124\times10^{-3}T - 0.917\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.705\times10^{-3}T + 0.062\times10^{-6}T^2 + 0.917\times10^{2}T^{-1} - 2.908$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr^\circ = -26.438 - 0.881\times10^{-3}T + 0.134\times10^{-6}T^2 + 11.500T^{-1}$

$\Delta Gr^\circ = -26.438 + 0.881\times10^{-3}T\ln T - 0.134\times10^{-6}T^2 + 5.750T^{-1} - 8.214\times10^{-3}T$

Source: Data are estimations from Mills (159).

$SeF_2(g)$

Selenium Difluoride (ideal gas)

[Reaction: $0.5Se_2(g) + F_2(g) = SeF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15*	11.400	64.440	64.440	0	-91.350	-87.443	64.097
300	11.420	64.510	64.443	.020	-91.353	-87.420	63.685
400	12.400	67.960	64.908	1.221	-91.418	-86.098	47.041
500	13.860	70.780	65.806	2.487	-91.460	-84.761	37.049
600	13.120	73.150	66.838	3.787	-91.496	-83.420	30.385
700	13.290	75.190	67.893	5.108	-91.528	-82.073	25.624
800	13.400	76.970	68.916	6.443	-91.559	-80.717	22.051
900	13.480	78.550	69.898	7.787	-91.588	-79.358	19.270
1000	13.550	79.980	70.841	9.139	-91.616	-78.006	17.048
1100	13.600	81.270	71.728	10.496	-91.641	-76.637	15.226
1200	13.640	82.460	72.578	11.858	-91.664	-75.278	13.710
1300	13.680	83.550	73.378	13.224	-91.685	-73.905	12.424
1400	13.720	84.560	74.136	14.594	-91.703	-72.533	11.323
1500	13.750	85.510	74.865	15.968	-91.718	-71.167	10.369
1600	13.780	86.400	75.560	17.344	-91.730	-69.801	9.534
1700	13.810	87.240	76.226	18.723	-91.739	-68.429	8.797
1800	13.830	88.030	76.861	20.105	-91.745	-67.062	8.142
1900	13.860	88.770	77.460	21.489	-91.748	-65.676	7.554
2000	13.880	89.490	78.052	22.876	-91.748	-64.324	7.029

*Data estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.568 + 0.178\times10^{-3}T - 1.974\times10^{5}T^{-2}$

$H°- H°_{298} = 13.568\times10^{-3}T + 0.089\times10^{-6}T^{2} + 1.974\times10^{2}T^{-1} - 4.715$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr° = -91.500 - 0.272\times10^{-3}T + 0.075\times10^{-6}T^{2} + 66.950T^{-1}$

$\Delta Gr° = -91.500 + 0.272\times10^{-3}T\ln T - 0.075\times10^{-6}T^{2} + 33.475T^{-1} + 11.702\times10^{-3}T$

Source: Data are estimations from Mills (159).

$SeF_4(g)$

Selenium Tetrafluoride (ideal gas)

[Reaction: $0.5Se_2(g) + 2F_2(g) = SeF_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	17.000	70.850	70.850	0	-210.650	-194.211	142.359
300	17.060	70.960	70.853	.032	-210.655	-194.111	141.408
400	20.390	76.400	71.573	1.931	-210.792	-188.568	103.027
500	21.960	81.140	73.028	4.056	-210.779	-183.013	79.994
600	22.850	85.230	74.728	6.301	-210.699	-177.468	64.642
700	23.420	88.790	76.481	8.616	-210.585	-171.932	53.679
800	23.830	91.950	78.225	10.980	-210.449	-166.422	45.464
900	24.130	94.770	79.906	13.378	-210.295	-160.923	39.077
1000	24.370	97.330	81.526	15.804	-210.128	-155.453	33.974
1100	24.580	99.660	83.067	18.252	-209.950	-149.989	29.800
1200	24.750	101.810	84.545	20.718	-209.760	-144.551	26.326
1300	24.910	103.800	85.953	23.201	-209.558	-139.125	23.389
1400	25.050	105.650	87.294	25.699	-209.348	-133.719	20.874
1500	25.180	107.380	88.573	28.211	-209.128	-128.320	18.696
1600	25.300	109.010	89.801	30.735	-208.898	-122.943	16.793
1700	25.420	110.550	90.979	33.271	-208.658	-117.574	15.115
1800	25.530	112.000	92.101	35.819	-208.411	-112.217	13.625
1900	25.640	113.390	93.191	38.378	-208.151	-106.892	12.295
2000	25.750	114.700	94.226	40.948	-207.885	-101.557	11.097

Phase change: 380.9 K, boiling point of SeF_4; $\Delta H°$ vaporization at 298 K = 10.8 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 24.167 + 0.870\times10^{-3}T - 6.602\times10^{5}T^{-2}$

$H°- H°_{298} = 24.167\times10^{-3}T + 0.435\times10^{-6}T^{2} + 6.602\times10^{2}T^{-1} - 9.458$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr° = -212.654 + 1.819\times10^{-3}T + 0.247\times10^{-6}T^{2} + 429.250T^{-1}$

$\Delta Gr° = -212.654 - 1.819\times10^{-3}T\ln T - 0.247\times10^{-6}T^{2} + 214.625T^{-1} + 69.880\times10^{-3}T$

Source: Data from Mills (159).

$SeF_5(g)$

Selenium Pentafluoride (ideal gas)

[Reaction: $0.5Se_2(g) + 2.5F_2(g) = SeF_5(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15*	22.800	76.990	76.990	0	-241.450	-219.620	160.984
300	22.870	77.130	76.990	.042	-241.452	-219.485	159.893
400	26.390	84.280	77.942	2.535	-241.379	-212.167	115.921
500	28.040	90.370	79.840	5.265	-241.163	-204.889	89.556
600	28.970	95.570	82.038	8.119	-240.889	-197.661	71.997
700	29.550	100.080	84.299	11.047	-240.587	-190.477	59.469
800	29.950	104.050	86.520	14.024	-240.269	-183.337	50.085
900	30.250	107.600	88.672	17.035	-239.937	-176.242	42.797
1000	30.480	110.800	90.728	20.072	-239.600	-169.187	36.975
1100	30.670	113.720	92.693	23.130	-239.253	-162.165	32.219
1200	30.830	116.390	94.552	26.206	-238.899	-155.166	28.259
1300	30.970	118.860	96.325	29.296	-238.538	-148.194	24.913
1400	31.100	121.160	98.017	32.400	-238.173	-141.265	22.052
1500	31.210	123.310	99.633	35.515	-237.801	-134.357	19.576
1600	31.320	125.330	101.179	38.642	-237.421	-127.477	17.412
1700	31.410	127.230	102.655	41.778	-237.035	-120.606	15.505
1800	31.510	129.030	104.072	44.924	-236.645	-113.777	13.814
1900	31.600	130.740	105.435	48.080	-236.245	-106.969	12.304
2000	31.680	132.360	106.738	51.244	-235.844	-100.173	10.946

*Data estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 30.544 + 0.652\times10^{-3}T - 7.056\times10^{5}T^{-2}$

$H°- H°_{298} = 30.544\times10^{-3}T + 0.326\times10^{-6}T^{2} + 7.056\times10^{2}T^{-1} - 11.502$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr° = -244.053 + 3.942\times10^{-3}T + 0.051\times10^{-6}T^{2} + 424.400T^{-1}$

$\Delta Gr° = -244.053 - 3.942\times10^{-3}T\ln T - 0.051\times10^{-6}T^{2} + 212.200T^{-1} + 102.037\times10^{-3}T$

Source: Data are estimations from Mills (159).

$SeF_6(g)$

Selenium Hexafluoride (ideal gas)

[Reaction: $0.5Se_2(g) + 3F_2(g) = SeF_6(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15	26.310	74.920	74.920	0	-283.600	-253.931	186.134
300	26.400	75.080	74.920	.049	-283.602	-253.747	184.852
400	30.880	83.400	76.025	2.950	-283.505	-243.801	133.205
500	32.980	90.540	78.232	6.154	-283.218	-233.906	102.239
600	34.150	96.670	80.812	9.515	-282.852	-224.082	81.621
700	34.900	101.990	83.461	12.970	-282.446	-214.314	66.911
800	35.410	106.690	86.081	16.487	-282.019	-204.614	55.897
900	35.790	110.880	88.603	20.049	-281.572	-194.959	47.342
1000	36.090	114.670	91.027	23.643	-281.118	-185.368	40.512
1100	36.330	118.120	93.335	27.264	-280.652	-175.811	34.930
1200	36.530	121.290	95.534	30.907	-280.176	-166.302	30.287
1300	36.710	124.220	97.628	34.570	-279.689	-156.825	26.364
1400	36.870	126.950	99.629	38.249	-279.199	-147.404	23.010
1500	37.010	129.500	101.538	41.943	-278.699	-138.010	20.108
1600	37.150	131.890	103.358	45.651	-278.192	-128.643	17.572
1700	37.270	134.140	105.098	49.372	-277.674	-119.292	15.336
1800	37.390	136.280	106.777	53.105	-277.154	-110.007	13.357
1900	37.500	138.300	108.379	56.850	-276.621	-100.727	11.586
2000	37.610	140.230	109.927	60.605	-276.087	-91.495	9.998

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 36.156 + 0.836\times10^{-3}T - 8.974\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 36.156\times10^{-3}T + 0.418\times10^{-6}T^2 + 8.974\times10^{2}T^{-1} - 13.827$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr^\circ = -287.083 + 5.300\times10^{-3}T + 0.056\times10^{-6}T^2 + 565.950T^{-1}$

$\Delta Gr^\circ = -287.083 - 5.300\times10^{-3}T\ln T - 0.056\times10^{-6}T^2 + 282.975T^{-1} + 138.223\times10^{-3}T$

Source: Data from Mills (159).

SiBr(g)
Silicon Monobromide (ideal gas)
[Formation: $Si(c,l) + 0.5Br_2(l,g) = SiBr(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	9.257	59.107	59.107	0	56.200	45.342	-33.236
300	9.260	59.165	59.108	.017	56.191	45.275	-32.982
332.6	9.282	60.121	59.162	.319	56.041	44.096	-28.975
332.6	9.282	60.121	59.162	.319	52.508	44.096	-28.975
400	9.327	61.842	59.472	.948	52.495	42.389	-23.160
500	9.298	63.921	60.161	1.880	52.440	39.870	-17.427
600	9.259	65.613	60.935	2.807	52.351	37.362	-13.609
700	9.229	67.038	61.707	3.732	52.238	34.872	-10.888
800	9.209	68.269	62.451	4.654	52.108	32.403	-8.852
900	9.196	69.353	63.160	5.574	51.958	29.948	-7.272
1000	9.189	70.321	63.828	6.493	51.799	27.519	-6.014
1100	9.187	71.197	64.459	7.412	51.630	25.091	-4.985
1200	9.189	71.996	65.054	8.331	51.453	22.687	-4.132
1300	9.193	72.732	65.617	9.250	51.270	20.296	-3.412
1400	9.198	73.413	66.149	10.169	51.079	17.926	-2.798
1500	9.206	74.048	66.655	11.089	50.882	15.553	-2.266
1600	9.214	74.643	67.137	12.010	50.681	13.201	-1.803
1687	9.222	75.130	67.536	12.812	50.501	11.191	-1.450
1687	9.222	75.130	67.536	12.812	38.419	11.191	-1.450
1700	9.223	75.201	67.594	12.932	38.401	10.985	-1.412
1800	9.234	75.729	68.032	13.855	38.258	9.378	-1.139
1900	9.244	76.228	68.450	14.779	38.116	7.780	-.895
2000	9.256	76.703	68.851	15.704	37.974	6.179	-.675

*Enthalpy of formation at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.
1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 9.299 - 0.064\times10^{-3}T - 0.021\times10^{5}T^{-2}$

$H°- H°_{298} = 9.299\times10^{-3}T - 0.032\times10^{-6}T^{2} + 0.021\times10^{2}T^{-1} - 2.777$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = 58.171 - 5.425\times10^{-3}T - 0.333\times10^{-6}T^{2} - 96.400T^{-1}$

$\Delta Gf° = 58.171 + 5.425\times10^{-3}T\ln T + 0.333\times10^{-6}T^{2} - 48.200T^{-1} - 73.496\times10^{-3}T$

332.6-1687 K: $\Delta Hf° = 53.170 - 0.845\times10^{-3}T - 0.410\times10^{-6}T^{2} - 112.100T^{-1}$

$\Delta Gf° = 53.170 + 0.845\times10^{-3}T\ln T + 0.410\times10^{-6}T^{2} - 56.050T^{-1} - 31.819\times10^{-3}T$

1687-2000 K: $\Delta Hf° = 40.741 - 1.266\times10^{-3}T - 0.060\times10^{-6}T^{2} - 13.600T^{-1}$

$\Delta Gf° = 40.741 + 1.266\times10^{-3}T\ln T + 0.060\times10^{-6}T^{2} - 6.800T^{-1} - 27.004\times10^{-3}T$

Source: Data from Chase (24) who estimated enthalpy of formation at 298 K and some molecular constants.

$SiBr_2(g)$

Silicon Dibromide (ideal gas)

[Formation: $Si(c,l) + Br_2(l,g) = SiBr_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	12.820	72.924	72.924	0	-12.500	-22.054	16.166
300	12.831	73.003	72.924	.024	-12.518	-22.113	16.109
332.6	12.970	74.334	72.997	.445	-12.844	-23.139	15.204
332.6	12.970	74.334	72.997	.445	-19.909	-23.139	15.204
400	13.258	76.761	73.434	1.331	-19.960	-23.794	13.000
500	13.479	79.745	74.407	2.669	-20.050	-24.741	10.814
600	13.605	82.215	75.510	4.023	-20.156	-25.671	9.350
700	13.683	84.318	76.621	5.388	-20.275	-26.581	8.299
800	13.735	86.149	77.700	6.759	-20.404	-27.470	7.504
900	13.771	87.769	78.730	8.135	-20.547	-28.345	6.883
1000	13.797	89.221	79.708	9.513	-20.697	-29.196	6.381
1100	13.817	90.537	80.633	10.894	-20.855	-30.046	5.969
1200	13.831	91.740	81.510	12.276	-21.020	-30.874	5.623
1300	13.843	92.848	82.340	13.660	-21.191	-31.690	5.327
1400	13.852	93.874	83.128	15.045	-21.369	-32.485	5.071
1500	13.860	94.830	83.877	16.430	-21.555	-33.285	4.850
1600	13.866	95.725	84.589	17.817	-21.745	-34.062	4.653
1687	13.870	96.460	85.183	19.024	-21.916	-34.708	4.496
1687	13.870	96.460	85.183	19.024	-33.998	-34.708	4.496
1700	13.871	96.566	85.270	19.204	-34.015	-34.709	4.462
1800	13.875	97.358	85.919	20.591	-34.149	-34.741	4.218
1900	13.879	98.109	86.541	21.979	-34.283	-34.769	3.999
2000	13.882	98.821	87.137	23.367	-34.419	-34.799	3.803

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.826 + 0.050\times10^{-3}T - 0.908\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.826\times10^{-3}T + 0.025\times10^{-6}T^2 + 0.908\times10^{2}T^{-1} - 4.429$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -9.489 - 9.944\times10^{-3}T - 0.226\times10^{-6}T^2 - 7.700T^{-1}$

$\Delta Gf^\circ = -9.489 + 9.944\times10^{-3}T\ln T + 0.226\times10^{-6}T^2 - 3.850T^{-1} - 98.824\times10^{-3}T$

332.6-1687 K: $\Delta Hf^\circ = -19.490 - 0.783\times10^{-3}T - 0.381\times10^{-6}T^2 - 39.100T^{-1}$

$\Delta Gf^\circ = -19.490 + 0.783\times10^{-3}T\ln T + 0.381\times10^{-6}T^2 - 19.550T^{-1} - 15.469\times10^{-3}T$

1687-2000 K: $\Delta Hf^\circ = -31.919 - 1.204\times10^{-3}T - 0.030\times10^{-6}T^2 + 59.400T^{-1}$

$\Delta Gf^\circ = -31.919 + 1.204\times10^{-3}T\ln T + 0.030\times10^{-6}T^2 + 29.700T^{-1} - 10.655\times10^{-3}T$

Source: Data from Chase (24) who estimated most molecular constants.

$SiBr_3(g)$

Silicon Tribromide (ideal gas)

[Formation: $Si(c,l) + 1.5Br_2(l,g) = SiBr_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	17.825	84.050	84.050	0	-48.206	-55.654	40.795
300	17.845	84.160	84.050	.033	-48.231	-55.700	40.577
332.6	18.101	86.014	84.153	.619	-48.686	-56.488	37.118
332.6	18.101	86.014	84.153	.619	-59.284	-56.488	37.118
400	18.629	89.414	84.762	1.861	-59.274	-55.929	30.558
500	19.042	93.620	86.126	3.747	-59.257	-55.094	24.081
600	19.282	97.115	87.675	5.664	-59.243	-54.263	19.765
700	19.432	100.099	89.242	7.600	-59.238	-53.434	16.683
800	19.532	102.701	90.765	9.549	-59.237	-52.602	14.370
900	19.602	105.006	92.222	11.506	-59.248	-51.773	12.572
1000	19.652	107.074	93.605	13.469	-59.263	-50.934	11.131
1100	19.690	108.949	94.916	15.436	-59.286	-50.108	9.955
1200	19.718	110.663	96.158	17.406	-59.315	-49.272	8.973
1300	19.741	112.242	97.335	19.379	-59.349	-48.434	8.142
1400	19.759	113.706	98.453	21.354	-59.390	-47.588	7.429
1500	19.773	115.070	99.516	23.331	-59.438	-46.756	6.812
1600	19.785	116.346	100.528	25.309	-59.492	-45.908	6.271
1687	19.794	117.394	101.371	27.031	-59.543	-45.150	5.849
1687	19.794	117.394	101.371	27.031	-71.625	-45.150	5.849
1700	19.795	117.546	101.494	27.288	-71.625	-44.941	5.778
1800	19.803	118.678	102.418	29.268	-71.621	-43.369	5.266
1900	19.810	119.749	103.303	31.248	-71.619	-41.798	4.808
2000	19.816	120.765	104.150	33.230	-71.618	-40.235	4.397

*Data estimated.

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.
1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.683 + 0.110\times10^{-3}T - 1.681\times10^{5}T^{-2}$

$H°- H°_{298} = 19.683\times10^{-3}T + 0.055\times10^{-6}T^2 + 1.681\times10^{2}T^{-1} - 6.437$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -44.511 - 13.132\times10^{-3}T - 0.146\times10^{-6}T^2 + 69.600T^{-1}$

$\Delta Gf° = -44.511 + 13.132\times10^{-3}T\ln T + 0.146\times10^{-6}T^2 + 34.800T^{-1} - 112.633\times10^{-3}T$

332.6-1687 K: $\Delta Hf° = -59.512 + 0.609\times10^{-3}T - 0.379\times10^{-6}T^2 + 22.500T^{-1}$

$\Delta Gf° = -59.512 - 0.609\times10^{-3}T\ln T + 0.379\times10^{-6}T^2 + 11.250T^{-1} + 12.399\times10^{-3}T$

1687-2000 K: $\Delta Hf° = -71.941 + 0.188\times10^{-3}T - 0.027\times10^{-6}T^2 + 121.000T^{-1}$

$\Delta Gf° = -71.941 - 0.188\times10^{-3}T\ln T + 0.027\times10^{-6}T^2 + 60.500T^{-1} + 17.213\times10^{-3}T$

Source: Data are those estimated by Chase (24).

$SiBr_4$(l,g)
Silicon Tetrabromide
[Formation: $Si(c,l) + 2Br_2(l,g) = SiBr_4(l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	35.000	66.500	66.500	0	-109.300	-106.093	77.767
300	35.000	66.717	66.500	.065	-109.310	-106.071	77.272
332.6	35.000	70.328	66.702	1.206	-109.504	-105.711	69.461
332.6	35.000	70.328	66.702	1.206	-123.634	-105.711	69.461
400	35.000	76.785	67.873	3.565	-122.801	-102.165	55.820
425.6	35.000	78.956	68.474	4.461	-122.492	-100.854	51.789
425.6	24.352	99.123	68.474	13.044	-113.909	-100.854	51.789
500	24.749	103.084	73.342	14.871	-113.805	-98.583	43.090
600	25.061	107.626	78.689	17.362	-113.662	-95.553	34.805
700	25.257	111.505	83.106	19.879	-113.522	-92.547	28.894
800	25.387	114.887	86.872	22.412	-113.384	-89.556	24.465
900	25.478	117.883	90.155	24.955	-113.259	-86.588	21.026
1000	25.544	120.571	93.065	27.506	-113.136	-83.623	18.276
1100	25.594	123.008	95.678	30.063	-113.020	-80.684	16.030
1200	25.631	125.236	98.049	32.625	-112.908	-77.748	14.160
1300	25.661	127.289	100.221	35.189	-112.804	-74.825	12.579
1400	25.684	129.192	102.223	37.757	-112.705	-71.901	11.224
1500	25.703	130.964	104.080	40.326	-112.615	-69.001	10.053
1600	25.719	132.624	105.813	42.897	-112.530	-66.098	9.028
1687	25.730	133.985	107.231	45.135	-112.461	-63.554	8.233
1687	25.730	133.985	107.231	45.135	-124.543	-63.554	8.233
1700	25.732	134.183	107.436	45.470	-124.524	-63.081	8.109
1800	25.743	135.654	108.963	48.044	-124.382	-59.467	7.220
1900	25.752	137.046	110.405	50.618	-124.242	-55.861	6.425
2000	25.760	138.368	111.771	53.194	-124.104	-52.276	5.712

Phase changes: 278.4 K, melting point of $SiBr_4$; ΔH° unknown.
332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
425.6 K, boiling point of $SiBr_4$; ΔH° = 8.583 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-425.6 K: $Cp° = 35.000$

$H°- H°_{298} = 35.000\times10^{-3}T - 10.435$

425.6-2000 K: $Cp° = 25.740 + 0.054\times10^{-3}T - 2.555\times10^{5}T^{-2}$

$H°- H°_{298} = 25.740\times10^{-3}T + 0.027\times10^{-6}T^2 + 2.555\times10^{2}T^{-1} + 1.484$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -106.911 - 6.861\times10^{-3}T - 0.151\times10^{-6}T^2 - 98.500T^{-1}$

$\Delta Gf° = -106.911 + 6.861\times10^{-3}T\ln T + 0.151\times10^{-6}T^2 - 49.250T^{-1} - 35.838\times10^{-3}T$

332.6-425.6 K: $\Delta Hf° = -126.911 + 11.461\times10^{-3}T - 0.461\times10^{-6}T^2 - 161.300T^{-1}$

$\Delta Gf° = -126.911 - 11.461\times10^{-3}T\ln T + 0.461\times10^{-6}T^2 - 80.650T^{-1} + 130.872\times10^{-3}T$

425.6-1687 K: $\Delta Hf° = -114.993 + 2.201\times10^{-3}T - 0.434\times10^{-6}T^2 + 94.200T^{-1}$

$\Delta Gf° = -114.993 - 2.201\times10^{-3}T\ln T + 0.434\times10^{-6}T^2 + 47.100T^{-1} + 46.118\times10^{-3}T$

1687-2000 K: $\Delta Hf° = -127.422 + 1.780\times10^{-3}T - 0.083\times10^{-6}T^2 + 192.700T^{-1}$

$\Delta Gf° = -127.422 - 1.780\times10^{-3}T\ln T + 0.083\times10^{-6}T^2 + 96.350T^{-1} + 50.932\times10^{-3}T$

Source: Data from Chase (24).

$SiBr_4(g)$

Silicon Tetrabromide (ideal gas)

[Formation: $Si(c,l) + 2Br_2(l,g) = SiBr_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	23.185	90.643	90.643	0	-99.300	-103.291	75.713
300	23.211	90.786	90.643	.043	-99.332	-103.314	75.263
332.6	23.538	93.197	90.777	.805	-99.905	-103.718	68.152
332.6	23.538	93.197	90.777	.805	-114.035	-103.718	68.152
400	24.215	97.617	91.567	2.420	-113.946	-101.643	55.535
500	24.749	103.084	93.342	4.871	-113.805	-98.583	43.090
600	25.061	107.626	95.356	7.362	-113.662	-95.553	34.805
700	25.257	111.505	97.392	9.879	-113.522	-92.547	28.894
800	25.387	114.887	99.372	12.412	-113.384	-89.556	24.465
900	25.478	117.883	101.266	14.955	-113.259	-86.588	21.026
1000	25.544	120.571	103.065	17.506	-113.136	-83.623	18.276
1100	25.594	123.008	104.769	20.063	-113.020	-80.684	16.030
1200	25.631	125.236	106.382	22.625	-112.908	-77.748	14.160
1300	25.661	127.289	107.913	25.189	-112.804	-74.825	12.579
1400	25.684	129.192	109.366	27.757	-112.705	-71.901	11.224
1500	25.703	130.964	110.747	30.326	-112.615	-69.001	10.053
1600	25.719	132.624	112.063	32.897	-112.530	-66.098	9.028
1687	25.730	133.985	113.158	35.135	-112.461	-63.554	8.233
1687	25.730	133.985	113.158	35.135	-124.543	-63.554	8.233
1700	25.732	134.183	113.318	35.470	-124.524	-63.081	8.109
1800	25.743	135.654	114.518	38.044	-124.382	-59.467	7.220
1900	25.752	137.046	115.668	40.618	-124.242	-55.861	6.425
2000	25.760	138.368	116.771	43.194	-124.104	-52.276	5.712

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.
1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 25.562 + 0.160\times10^{-3}T - 2.155\times10^{5}T^{-2}$

$H°- H°_{298} = 25.562\times10^{-3}T + 0.080\times10^{-6}T^2 + 2.155\times10^{2}T^{-1} - 8.351$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -94.827 - 16.299\times10^{-3}T - 0.071\times10^{-6}T^2 + 117.000T^{-1}$

$\Delta Gf° = -94.827 + 16.299\times10^{-3}T\ln T + 0.071\times10^{-6}T^2 + 58.500T^{-1} - 121.933\times10^{-3}T$

332.6-1687 K: $\Delta Hf° = -114.827 + 2.023\times10^{-3}T - 0.381\times10^{-6}T^2 + 54.200T^{-1}$

$\Delta Gf° = -114.827 - 2.023\times10^{-3}T\ln T + 0.381\times10^{-6}T^2 + 27.100T^{-1} + 44.777\times10^{-3}T$

1687-2000 K: $\Delta Hf° = -127.256 + 1.602\times10^{-3}T - 0.030\times10^{-6}T^2 + 152.700T^{-1}$

$\Delta Gf° = -127.256 - 1.602\times10^{-3}T\ln T + 0.030\times10^{-6}T^2 + 76.350T^{-1} + 49.591\times10^{-3}T$

Source: Data from Chase (24).

SiCl(g)
Silicon Monochloride (ideal gas)
[Formation: $Si(c,l) + 0.5Cl_2(g) = SiCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.551	56.816	56.816	0	47.400	39.746	-29.134
300	8.555	56.869	56.816	.016	47.400	39.699	-28.920
400	8.710	59.354	57.154	.880	47.342	37.137	-20.290
500	8.803	61.308	57.796	1.756	47.245	34.598	-15.123
600	8.864	62.919	58.521	2.639	47.122	32.078	-11.684
700	8.907	64.289	59.249	3.528	46.981	29.581	-9.236
800	8.938	65.480	59.955	4.420	46.825	27.108	-7.405
900	8.964	66.534	60.628	5.315	46.654	24.654	-5.987
1000	8.984	67.480	61.267	6.213	46.478	22.227	-4.858
1100	9.002	68.337	61.872	7.112	46.291	19.802	-3.934
1200	9.018	69.121	62.444	8.013	46.098	17.402	-3.169
1300	9.033	69.843	62.985	8.916	45.900	15.020	-2.525
1400	9.047	70.513	63.499	9.820	45.695	12.656	-1.976
1500	9.059	71.138	63.988	10.725	45.484	10.292	-1.499
1600	9.071	71.723	64.453	11.632	45.269	7.951	-1.086
1687	9.081	72.203	64.841	12.421	45.077	5.948	-.771
1687	9.081	72.203	64.841	12.421	32.995	5.948	-.771
1700	9.083	72.273	64.897	12.539	32.975	5.745	-.739
1800	9.094	72.793	65.322	13.448	32.818	4.149	-.504
1900	9.105	73.285	65.728	14.358	32.662	2.561	-.295
2000	9.116	73.752	66.118	15.269	32.506	.976	-.107

Phase change: 1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.865 + 0.140\times10^{-3}T - 0.316\times10^{5}T^{-2}$

$H°- H°_{298} = 8.865\times10^{-3}T + 0.070\times10^{-6}T^{2} + 0.316\times10^{2}T^{-1} - 2.755$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = 48.134 - 1.227\times10^{-3}T - 0.325\times10^{-6}T^{2} - 101.050T^{-1}$

$\Delta Gf° = 48.134 + 1.227\times10^{-3}T\ln T + 0.325\times10^{-6}T^{2} - 50.525T^{-1} - 34.654\times10^{-3}T$

1687-2000 K: $\Delta Hf° = 35.705 - 1.649\times10^{-3}T + 0.026\times10^{-6}T^{2} - 2.550T^{-1}$

$\Delta Gf° = 35.705 + 1.649\times10^{-3}T\ln T - 0.026\times10^{-6}T^{2} - 1.275T^{-1} - 29.840\times10^{-3}T$

Source: Data from Chase (24).

$SiCl_2(g)$

Silicon Dichloride (ideal gas)

[Formation: $Si(c,l) + Cl_2(g) = SiCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	12.248	67.214	67.214	0	-40.300	-43.110	31.600
300	12.264	67.290	67.214	.023	-40.301	-43.127	31.418
400	12.881	70.912	67.705	1.283	-40.378	-44.061	24.073
500	13.216	73.826	68.646	2.590	-40.470	-44.968	19.655
600	13.414	76.254	69.717	3.922	-40.579	-45.860	16.704
700	13.539	78.332	70.803	5.270	-40.700	-46.731	14.590
800	13.623	80.146	71.861	6.628	-40.833	-47.583	12.999
900	13.681	81.754	72.872	7.994	-40.977	-48.417	11.757
1000	13.724	83.198	73.834	9.364	-41.129	-49.229	10.759
1100	13.756	84.507	74.745	10.738	-41.289	-50.038	9.942
1200	13.780	85.705	75.609	12.115	-41.456	-50.827	9.257
1300	13.799	86.809	76.429	13.494	-41.629	-51.601	8.675
1400	13.814	87.832	77.207	14.875	-41.809	-52.357	8.173
1500	13.826	88.786	77.948	16.257	-41.996	-53.116	7.739
1600	13.836	89.678	78.653	17.640	-42.189	-53.851	7.356
1687	13.844	90.412	79.242	18.844	-42.362	-54.460	7.055
1687	13.844	90.412	79.242	18.844	-54.444	-54.460	7.055
1700	13.845	90.518	79.327	19.024	-54.461	-54.456	7.001
1800	13.852	91.309	79.971	20.409	-54.597	-54.449	6.611
1900	13.858	92.058	80.587	21.794	-54.734	-54.436	6.261
2000	13.863	92.769	81.179	23.180	-54.873	-54.423	5.947

Phase change: 1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.694 + 0.134\times10^{-3}T - 1.321\times10^{5}T^{-2}$

$H°- H°_{298} = 13.694\times10^{-3}T + 0.067\times10^{-6}T^{2} + 1.321\times10^{2}T^{-1} - 4.532$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = -39.908 - 0.812\times10^{-3}T - 0.372\times10^{-6}T^{2} - 34.700T^{-1}$

$\Delta Gf° = -39.908 + 0.812\times10^{-3}T\ln T + 0.372\times10^{-6}T^{2} - 17.350T^{-1} - 15.279\times10^{-3}T$

1687-2000 K: $\Delta Hf° = -52.338 - 1.233\times10^{-3}T - 0.021\times10^{-6}T^{2} + 63.800T^{-1}$

$\Delta Gf° = -52.338 + 1.233\times10^{-3}T\ln T + 0.021\times10^{-6}T^{2} + 31.900T^{-1} - 10.465\times10^{-3}T$

Source: Data from Chase (24).

$SiCl_3(g)$

Silicon Trichloride (ideal gas)

[Formation: $Si(c,1) + 1.5Cl_2(g) = SiCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	16.906	76.023	76.023	0	-93.300	-90.792	66.551
300	16.933	76.127	76.024	.031	-93.301	-90.777	66.130
400	18.015	81.163	76.703	1.784	-93.300	-89.938	49.139
500	18.613	85.253	78.017	3.618	-93.291	-89.096	38.943
600	18.969	88.681	79.516	5.499	-93.285	-88.258	32.148
700	19.195	91.623	81.040	7.408	-93.285	-87.421	27.294
800	19.347	94.197	82.527	9.336	-93.291	-86.583	23.653
900	19.453	96.482	83.953	11.276	-93.306	-85.742	20.821
1000	19.530	98.536	85.311	13.225	-93.326	-84.895	18.553
1100	19.588	100.400	86.599	15.181	-93.352	-84.058	16.700
1200	19.633	102.107	87.822	17.142	-93.385	-83.213	15.155
1300	19.668	103.679	88.981	19.107	-93.423	-82.363	13.846
1400	19.695	105.138	90.084	21.076	-93.467	-81.505	12.723
1500	19.718	106.498	91.134	23.046	-93.519	-80.662	11.752
1600	19.736	107.771	92.134	25.019	-93.576	-79.804	10.901
1687	19.750	108.816	92.968	26.736	-93.631	-79.030	10.238
1687	19.750	108.816	92.968	26.736	-105.713	-79.030	10.238
1700	19.752	108.968	93.090	26.993	-105.713	-78.821	10.133
1800	19.764	110.097	94.003	28.969	-105.713	-77.238	9.378
1900	19.775	111.166	94.879	30.946	-105.714	-75.653	8.702
2000	19.785	112.181	95.719	32.924	-105.719	-74.078	8.095

Phase change: 1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.453 + 0.252\times10^{-3}T - 2.331\times10^{5}T^{-2}$

$H°- H°_{298} = 19.453\times10^{-3}T + 0.126\times10^{-6}T^2 + 2.331\times10^{2}T^{-1} - 6.593$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = -93.535 + 0.533\times10^{-3}T - 0.357\times10^{-6}T^2 + 32.150T^{-1}$

$\Delta Gf° = -93.535 - 0.533\times10^{-3}T\ln T + 0.357\times10^{-6}T^2 + 16.075T^{-1} + 11.953\times10^{-3}T$

1687-2000 K: $\Delta Hf° = -105.964 + 0.112\times10^{-3}T - 0.006\times10^{-6}T^2 + 130.650T^{-1}$

$\Delta Gf° = -105.964 - 0.112\times10^{-3}T\ln T + 0.006\times10^{-6}T^2 + 65.325T^{-1} + 16.767\times10^{-3}T$

Source: Data from Chase (24) who estimated some molecular constants.

$SiCl_4(g)$

Silicon Tetrachloride (ideal gas)

[Formation: $Si(c,l) + 2Cl_2(g) = SiCl_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	21.573	79.070	79.070	0	-158.400	-148.856	109.113
300	21.610	79.204	79.071	.040	-158.399	-148.797	108.397
400	23.133	85.651	79.938	2.285	-158.321	-145.609	79.556
500	23.989	90.914	81.624	4.645	-158.213	-142.441	62.260
600	24.505	95.337	83.552	7.071	-158.097	-139.300	50.739
700	24.835	99.141	85.514	9.539	-157.976	-136.177	42.516
800	25.057	102.473	87.429	12.035	-157.857	-133.071	36.353
900	25.214	105.433	89.267	14.549	-157.743	-129.977	31.562
1000	25.328	108.096	91.020	17.076	-157.632	-126.892	27.732
1100	25.413	110.514	92.684	19.613	-157.526	-123.831	24.603
1200	25.479	112.728	94.263	22.158	-157.425	-120.772	21.995
1300	25.530	114.770	95.763	24.709	-157.328	-117.722	19.791
1400	25.571	116.663	97.189	27.264	-157.238	-114.674	17.901
1500	25.604	118.429	98.547	29.823	-157.154	-111.649	16.267
1600	25.632	120.082	99.842	32.384	-157.077	-108.619	14.837
1687	25.651	121.440	100.921	34.616	-157.013	-105.962	13.727
1687	25.651	121.440	100.921	34.616	-169.095	-105.962	13.727
1700	25.654	121.637	101.079	34.949	-169.077	-105.471	13.559
1800	25.674	123.104	102.262	37.515	-168.943	-101.735	12.352
1900	25.690	124.492	103.396	40.083	-168.809	-98.000	11.272
2000	25.704	125.810	104.483	42.653	-168.679	-94.283	10.303

Phase change: 1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 25.159 + 0.406\times10^{-3}T - 3.295\times10^{5}T^{-2}$

$H°- H°_{298} = 25.159\times10^{-3}T + 0.203\times10^{-6}T^2 + 3.295\times10^{2}T^{-1} - 8.624$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = -159.232 + 1.826\times10^{-3}T - 0.324\times10^{-6}T^2 + 94.400T^{-1}$

$\Delta Gf° = -159.232 - 1.826\times10^{-3}T\ln T + 0.324\times10^{-6}T^2 + 47.200T^{-1} + 44.578\times10^{-3}T$

1687-2000 K: $\Delta Hf° = -171.661 + 1.405\times10^{-3}T + 0.027\times10^{-6}T^2 + 192.900T^{-1}$

$\Delta Gf° = -171.661 - 1.405\times10^{-3}T\ln T - 0.027\times10^{-6}T^2 + 96.450T^{-1} + 49.392\times10^{-3}T$

Source: Data from Chase (25).

SiF(g)

Silicon Monofluoride (ideal gas)

[Formation: $Si(c,l) + 0.5F_2(g) = SiF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	7.803	53.937	53.937	0	-4.800	-12.318	9.029
300	7.809	53.985	53.938	.014	-4.802	-12.365	9.008
400	8.096	56.272	54.247	.810	-4.898	-14.874	8.127
500	8.326	58.104	54.840	1.632	-5.024	-17.352	7.585
600	8.492	59.638	55.516	2.473	-5.170	-19.807	7.215
700	8.611	60.956	56.202	3.328	-5.330	-22.235	6.942
800	8.699	62.112	56.869	4.194	-5.500	-24.636	6.730
900	8.765	63.141	57.511	5.067	-5.682	-27.018	6.561
1000	8.817	64.067	58.120	5.947	-5.870	-29.370	6.419
1100	8.859	64.910	58.700	6.831	-6.066	-31.718	6.302
1200	8.893	65.682	59.250	7.718	-6.269	-34.042	6.200
1300	8.922	66.395	59.773	8.609	-6.475	-36.348	6.111
1400	8.946	67.057	60.270	9.502	-6.689	-38.634	6.031
1500	8.968	67.675	60.743	10.398	-6.908	-40.919	5.962
1600	8.988	68.254	61.194	11.296	-7.131	-43.180	5.898
1687	9.003	68.731	61.571	12.079	-7.328	-45.114	5.844
1687	9.003	68.731	61.571	12.079	-19.410	-45.114	5.844
1700	9.005	68.800	61.626	12.196	-19.431	-45.308	5.825
1800	9.021	69.315	62.039	13.097	-19.597	-46.823	5.685
1900	9.036	69.803	62.435	14.000	-19.760	-48.330	5.559
2000	9.050	70.267	62.815	14.904	-19.924	-49.836	5.446

Phase change: 1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.440 + 0.380\times10^{-3}T - 0.667\times10^{5}T^{-2}$

$H°- H°_{298} = 8.440\times10^{-3}T + 0.190\times10^{-6}T^{2} + 0.667\times10^{2}T^{-1} - 2.757$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = -4.058 - 1.493\times10^{-3}T - 0.248\times10^{-6}T^{2} - 82.050T^{-1}$

$\Delta Gf° = -4.058 + 1.493\times10^{-3}T\ln T + 0.248\times10^{-6}T^{2} - 41.025T^{-1} - 35.824\times10^{-3}T$

1687-2000 K: $\Delta Hf° = -16.487 - 1.914\times10^{-3}T + 0.103\times10^{-6}T^{2} + 16.450T^{-1}$

$\Delta Gf° = -16.487 + 1.914\times10^{-3}T\ln T - 0.103\times10^{-6}T^{2} + 8.225T^{-1} - 31.010\times10^{-3}T$

Source: Data from Chase (24).

$SiF_2(g)$
Silicon Difluoride (ideal gas)
[Formation: $Si(c,l) + F_2(g) = SiF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	10.638	61.298	61.298	0	-140.500	-142.991	104.814
300	10.658	61.363	61.298	.020	-140.503	-143.006	104.179
400	11.581	64.564	61.729	1.134	-140.665	-143.819	78.578
500	12.214	67.221	62.569	2.326	-140.823	-144.587	63.198
600	12.640	69.488	63.538	3.570	-140.981	-145.327	52.935
700	12.932	71.459	64.530	4.850	-141.140	-146.038	45.595
800	13.137	73.200	65.507	6.154	-141.303	-146.725	40.083
900	13.285	74.757	66.451	7.475	-141.473	-147.393	35.791
1000	13.396	76.162	67.352	8.810	-141.646	-148.033	32.352
1100	13.480	77.443	68.212	10.154	-141.825	-148.670	29.538
1200	13.545	78.619	69.032	11.505	-142.009	-149.286	27.188
1300	13.597	79.705	69.811	12.862	-142.197	-149.884	25.197
1400	13.639	80.715	70.555	14.224	-142.392	-150.466	23.488
1500	13.673	81.657	71.264	15.590	-142.592	-151.046	22.007
1600	13.701	82.540	71.941	16.958	-142.798	-151.604	20.708
1687	13.721	83.267	72.507	18.152	-142.980	-152.056	19.699
1687	13.721	83.267	72.507	18.152	-155.062	-152.056	19.699
1700	13.724	83.372	72.590	18.330	-155.081	-152.029	19.544
1800	13.744	84.157	73.211	19.703	-155.230	-151.844	18.436
1900	13.760	84.900	73.806	21.078	-155.378	-151.650	17.444
2000	13.775	85.606	74.379	22.455	-155.528	-151.456	16.550

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 12.817 + 0.650\times10^{-3}T - 2.109\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 12.817\times10^{-3}T + 0.325\times10^{-6}T^2 + 2.109\times10^{2}T^{-1} - 4.558$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf^\circ = -140.114 - 1.370\times10^{-3}T - 0.200\times10^{-6}T^2 + 11.900T^{-1}$

$\Delta Gf^\circ = -140.114 + 1.370\times10^{-3}T\ln T + 0.200\times10^{-6}T^2 + 5.950T^{-1} - 17.583\times10^{-3}T$

1687-2000 K: $\Delta Hf^\circ = -152.543 - 1.791\times10^{-3}T + 0.151\times10^{-6}T^2 + 110.400T^{-1}$

$\Delta Gf^\circ = -152.543 + 1.791\times10^{-3}T\ln T - 0.151\times10^{-6}T^2 + 55.200T^{-1} - 12.769\times10^{-3}T$

Source: Data from Chase (24).

$SiF_3(g)$
Silicon Trifluoride (ideal gas)
[Formation: $Si(c,l) + 1.5F_2(g) = SiF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	14.251	67.464	67.464	0	-259.400	-256.508	188.023
300	14.285	67.553	67.466	.026	-259.404	-256.491	186.851
400	15.856	71.891	68.046	1.538	-259.552	-255.497	139.595
500	16.932	75.552	69.190	3.181	-259.661	-254.468	111.226
600	17.660	78.708	70.520	4.913	-259.746	-253.423	92.308
700	18.162	81.470	71.890	6.706	-259.816	-252.363	78.790
800	18.518	83.920	73.244	8.541	-259.879	-251.293	68.649
900	18.776	86.117	74.555	10.406	-259.941	-250.215	60.760
1000	18.969	88.105	75.811	12.294	-260.001	-249.123	54.445
1100	19.116	89.921	77.014	14.198	-260.063	-248.041	49.281
1200	19.230	91.589	78.159	16.116	-260.125	-246.945	44.974
1300	19.321	93.132	79.253	18.043	-260.191	-245.844	41.330
1400	19.394	94.566	80.295	19.979	-260.262	-244.735	38.204
1500	19.453	95.907	81.292	21.922	-260.336	-243.635	35.497
1600	19.502	97.164	82.246	23.869	-260.417	-242.520	33.126
1687	19.538	98.197	83.041	25.568	-260.488	-241.522	31.289
1687	19.538	98.197	83.041	25.568	-272.570	-241.522	31.289
1700	19.543	98.347	83.158	25.822	-272.572	-241.278	31.018
1800	19.578	99.465	84.033	27.778	-272.595	-239.435	29.071
1900	19.608	100.525	84.874	29.737	-272.615	-237.592	27.329
2000	19.633	101.531	85.681	31.699	-272.638	-235.754	25.762

Phase change: 1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 17.940 + 1.142\times10^{-3}T - 3.583\times10^{5}T^{-2}$

$H°- H°_{298} = 17.940\times10^{-3}T + 0.571\times10^{-6}T^2 + 3.583\times10^{2}T^{-1} - 6.601$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = -259.613 - 0.501\times10^{-3}T - 0.041\times10^{-6}T^2 + 109.050T^{-1}$

$\Delta Gf° = -259.613 + 0.501\times10^{-3}T\ln T + 0.041\times10^{-6}T^2 + 54.525T^{-1} + 6.934\times10^{-3}T$

1687-2000 K: $\Delta Hf° = -272.042 - 0.922\times10^{-3}T + 0.310\times10^{-6}T^2 + 207.550T^{-1}$

$\Delta Gf° = -272.042 + 0.922\times10^{-3}T\ln T - 0.310\times10^{-6}T^2 + 103.775T^{-1} + 11.748\times10^{-3}T$

Source: Data from Chase (24) who estimated some molecular constants.

$SiF_4(g)$

Silicon Tetrafluoride (ideal gas)

[Formation: $Si(c,l) + 2F_2(g) = SiF_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	17.596	67.554	67.554	0	-385.980	-375.893	275.533
300	17.644	67.663	67.554	.033	-385.984	-375.831	273.789
400	19.871	73.062	68.274	1.915	-386.147	-372.420	203.478
500	21.421	77.673	69.705	3.984	-386.232	-368.975	161.277
600	22.488	81.679	71.374	6.183	-386.265	-365.522	133.140
700	23.233	85.205	73.104	8.471	-386.264	-362.066	113.041
800	23.765	88.344	74.817	10.822	-386.242	-358.610	97.966
900	24.154	91.167	76.479	13.219	-386.207	-355.156	86.243
1000	24.446	93.727	78.077	15.650	-386.164	-351.701	76.863
1100	24.670	96.068	79.608	18.106	-386.117	-348.264	69.193
1200	24.845	98.223	81.071	20.582	-386.067	-344.827	62.801
1300	24.983	100.217	82.468	23.074	-386.015	-341.390	57.392
1400	25.095	102.073	83.803	25.578	-385.968	-337.958	52.757
1500	25.187	103.807	85.078	28.093	-385.922	-334.540	48.742
1600	25.262	105.435	86.301	30.615	-385.880	-331.117	45.228
1687	25.317	106.775	87.322	32.816	-385.845	-328.118	42.507
1687	25.317	106.775	87.322	32.816	-397.927	-328.118	42.507
1700	25.325	106.969	87.472	33.145	-397.913	-327.576	42.112
1800	25.379	108.418	88.596	35.680	-397.812	-323.440	39.270
1900	25.424	109.791	89.675	38.220	-397.708	-319.308	36.728
2000	25.463	111.096	90.714	40.764	-397.608	-315.192	34.442

Phase change: 1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 23.001 + 1.622\times10^{-3}T - 5.235\times10^{5}T^{-2}$

$H°- H°_{298} = 23.001\times10^{-3}T + 0.811\times10^{-5}T^{2} + 5.235\times10^{2}T^{-1} - 8.686$

Formation equations (kcal/mol):

298.15-1687 K: $\Delta Hf° = -386.833 + 0.306\times10^{-3}T + 0.112\times10^{-6}T^{2} + 224.000T^{-1}$

$\Delta Gf° = -386.833 - 0.306\times10^{-3}T\ln T - 0.112\times10^{-6}T^{2} + 112.000T^{-1} + 37.208\times10^{-3}T$

1687-2000 K: $\Delta Hf° = -399.262 - 0.115\times10^{-3}T + 0.463\times10^{-6}T^{2} + 322.500T^{-1}$

$\Delta Gf° = -399.262 + 0.115\times10^{-3}T\ln T - 0.463\times10^{-6}T^{2} + 161.250T^{-1} + 42.022\times10^{-3}T$

Source: Data from Chase (26).

SiI(g)

Silicon Monoiodide (ideal gas)

[Formation: $Si(c,l) + 0.5I_2(c,l,g) = SiI(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	9.330	60.646	60.646	0	74.959	62.357	-45.708
300	9.339	60.703	60.646	.017	74.955	62.279	-45.370
386.8	9.580	63.115	60.940	.841	74.738	58.636	-33.130
386.8	9.580	63.115	60.940	.841	72.883	58.636	-33.130
400	9.617	63.437	61.017	.968	72.813	58.151	-31.772
458.4	9.637	64.751	61.410	1.532	72.499	56.035	-26.715
458.4	9.637	64.751	61.410	1.532	67.489	56.035	-26.715
500	9.651	65.589	61.723	1.933	67.473	54.997	-24.039
600	9.603	67.345	62.518	2.896	67.416	52.505	-19.125
700	9.537	68.821	63.317	3.853	67.332	50.025	-15.618
800	9.477	70.090	64.086	4.803	67.227	47.561	-12.993
900	9.427	71.203	64.816	5.748	67.100	45.110	-10.954
1000	9.387	72.194	65.505	6.689	66.960	42.684	-9.328
1100	9.357	73.087	66.154	7.626	66.806	40.255	-7.998
1200	9.335	73.901	66.767	8.561	66.643	37.848	-6.893
1300	9.319	74.647	67.345	9.493	66.471	35.455	-5.960
1400	9.307	75.337	67.891	10.425	66.290	33.082	-5.164
1500	9.300	75.979	68.409	11.355	66.100	30.704	-4.473
1600	9.296	76.579	68.901	12.285	65.905	28.350	-3.872
1687	9.295	77.072	69.310	13.093	65.729	26.332	-3.411
1687	9.295	77.072	69.310	13.093	53.647	26.332	-3.411
1700	9.295	77.143	69.370	13.214	53.629	26.126	-3.359
1800	9.296	77.674	69.816	14.144	53.490	24.515	-2.976
1900	9.299	78.177	70.243	15.074	53.351	22.909	-2.635
2000	9.303	78.654	70.652	16.004	53.211	21.305	-2.328

Phase changes: 386.8 K, melting point of I_2; $\Delta H° = 3.709$ kcal/mol.
458.4 K, boiling point of I_2; $\Delta H° = 10.021$ kcal/mol.
1687 K, melting point of Si; $\Delta H° = 12.082$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 9.953 - 0.424\times10^{-3}T - 0.442\times10^{5}T^{-2}$

$H°- H°_{298} = 9.953\times10^{-3}T - 0.212\times10^{-6}T^2 + 0.442\times10^{2}T^{-1} - 3.097$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = 75.903 - 2.164\times10^{-3}T - 1.309\times10^{-6}T^2 - 54.300T^{-1}$

$\Delta Gf° = 75.903 + 2.164\times10^{-3}T\ln T + 1.309\times10^{-6}T^2 - 27.150T^{-1} - 57.850\times10^{-3}T$

386.8-458.4 K: $\Delta Hf° = 75.175 - 5.367\times10^{-3}T - 0.563\times10^{-6}T^2 - 54.300T^{-1}$

$\Delta Gf° = 75.175 + 5.367\times10^{-3}T\ln T + 0.563\times10^{-6}T^2 - 27.150T^{-1} - 74.758\times10^{-3}T$

458.4-1687 K: $\Delta Hf° = 67.819 - 0.197\times10^{-3}T - 0.597\times10^{-6}T^2 - 61.950T^{-1}$

$\Delta Gf° = 67.819 + 0.197\times10^{-3}T\ln T + 0.597\times10^{-6}T^2 - 30.975T^{-1} - 27.026\times10^{-3}T$

1687-2000 K: $\Delta Hf° = 55.390 - 0.618\times10^{-3}T - 0.246\times10^{-6}T^2 + 36.550T^{-1}$

$\Delta Gf° = 55.390 + 0.618\times10^{-3}T\ln T + 0.246\times10^{-6}T^2 + 18.275T^{-1} - 22.212\times10^{-3}T$

Source: Data from Chase (24).

$SiI_2(g)$

Silicon Diiodide (ideal gas)

[Formation: $Si(c,l) + I_2(c,l,g) = SiI_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	13.055	76.688	76.688	0	22.100	8.853	-6.489
300	13.065	76.768	76.688	.024	22.091	8.771	-6.390
386.8	13.362	80.131	77.097	1.173	21.595	4.977	-2.812
386.8	13.362	80.131	77.097	1.173	17.886	4.977	-2.812
400	13.407	80.580	77.205	1.350	17.738	4.539	-2.480
458.4	13.508	82.415	77.755	2.137	17.084	2.661	-1.269
458.4	13.508	82.415	77.755	2.137	7.063	2.661	-1.269
500	13.580	83.592	78.192	2.700	7.024	2.264	-.990
600	13.677	86.078	79.306	4.063	6.918	1.319	-.481
700	13.738	88.191	80.428	5.434	6.799	.395	-.123
800	13.777	90.028	81.516	6.810	6.669	-.508	.139
900	13.805	91.652	82.553	8.189	6.524	-1.397	.339
1000	13.825	93.108	83.537	9.571	6.373	-2.260	.494
1100	13.839	94.426	84.468	10.954	6.212	-3.124	.621
1200	13.851	95.631	85.348	12.339	6.044	-3.965	.722
1300	13.859	96.740	86.183	13.724	5.870	-4.793	.806
1400	13.866	97.767	86.973	15.111	5.688	-5.600	.874
1500	13.872	98.724	87.726	16.497	5.498	-6.413	.934
1600	13.877	99.620	88.442	17.885	5.304	-7.202	.984
1687	13.880	100.354	89.037	19.093	5.129	-7.856	1.018
1687	13.880	100.354	89.037	19.093	-6.953	-7.856	1.018
1700	13.881	100.461	89.124	19.273	-6.971	-7.858	1.010
1800	13.884	101.254	89.776	20.661	-7.110	-7.904	.960
1900	13.887	102.005	90.400	22.050	-7.250	-7.943	.914
2000	13.889	102.718	90.999	23.438	-7.392	-7.984	.872

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.851 + 0.038\times10^{-3}T - 0.718\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.851\times10^{-3}T + 0.019\times10^{-6}T^2 + 0.718\times10^{2}T^{-1} - 4.372$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = 23.754 - 4.705\times10^{-3}T - 1.824\times10^{-6}T^2 - 26.700T^{-1}$

$\Delta Gf^\circ = 23.754 + 4.705\times10^{-3}T\ln T + 1.824\times10^{-6}T^2 - 13.350T^{-1} - 77.180\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = 22.299 - 11.109\times10^{-3}T - 0.332\times10^{-6}T^2 - 26.700T^{-1}$

$\Delta Gf^\circ = 22.299 + 11.109\times10^{-3}T\ln T + 0.332\times10^{-6}T^2 - 13.350T^{-1} - 110.995\times10^{-3}T$

458.4-1687 K: $\Delta Hf^\circ = 7.586 - 0.769\times10^{-3}T - 0.400\times10^{-6}T^2 - 42.000T^{-1}$

$\Delta Gf^\circ = 7.586 + 0.769\times10^{-3}T\ln T + 0.400\times10^{-6}T^2 - 21.000T^{-1} - 15.532\times10^{-3}T$

1687-2000 K: $\Delta Hf^\circ = -4.843 - 1.190\times10^{-3}T - 0.049\times10^{-6}T^2 + 56.500T^{-1}$

$\Delta Gf^\circ = -4.843 + 1.190\times10^{-3}T\ln T + 0.049\times10^{-6}T^2 + 28.250T^{-1} - 10.718\times10^{-3}T$

Source: Data from Chase (24) who estimated molecular constants.

$SiI_3(g)$

Silicon Triiodide (ideal gas)

[Formation: $Si(c,l) + 1.5I_2(c,l,g) = SiI_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	18.449	90.391	90.391	0	8.440	-4.754	3.485
300	18.464	90.505	90.392	.034	8.429	-4.836	3.523
386.8	18.954	95.267	90.972	1.661	7.807	-8.600	4.859
386.8	18.954	95.267	90.972	1.661	2.243	-8.600	4.859
400	19.029	95.904	91.124	1.912	2.042	-8.966	4.899
458.4	19.197	98.511	91.901	3.030	1.157	-10.507	5.009
458.4	19.197	98.511	91.901	3.030	-13.874	-10.507	5.009
500	19.316	100.184	92.522	3.831	-13.862	-10.199	4.458
600	19.480	103.722	94.102	5.772	-13.839	-9.471	3.450
700	19.581	106.733	95.697	7.725	-13.825	-8.745	2.730
800	19.648	109.352	97.243	9.687	-13.819	-8.017	2.190
900	19.694	111.669	98.720	11.654	-13.829	-7.292	1.771
1000	19.727	113.746	100.121	13.625	-13.843	-6.557	1.433
1100	19.752	115.627	101.446	15.599	-13.867	-5.835	1.159
1200	19.771	117.347	102.701	17.575	-13.898	-5.104	.930
1300	19.786	118.930	103.889	19.553	-13.933	-4.369	.735
1400	19.798	120.397	105.017	21.532	-13.979	-3.628	.566
1500	19.807	121.763	106.088	23.512	-14.032	-2.900	.422
1600	19.815	123.042	107.108	25.494	-14.089	-2.155	.294
1687	19.820	124.091	107.957	27.217	-14.147	-1.484	.192
1687	19.820	124.091	107.957	27.217	-26.229	-1.484	.192
1700	19.821	124.243	108.081	27.475	-26.229	-1.289	.166
1800	19.827	125.376	109.010	29.458	-26.232	.181	-.022
1900	19.831	126.448	109.900	31.441	-26.237	1.649	-.190
2000	19.835	127.466	110.754	33.424	-26.244	3.110	-.340

*Data estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.776 + 0.058\times10^{-3}T - 1.195\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.776\times10^{-3}T + 0.029\times10^{-6}T^2 + 1.195\times10^{2}T^{-1} - 6.300$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = 10.153 - 5.219\times10^{-3}T - 2.560\times10^{-6}T^2 + 21.000T^{-1}$

$\Delta Gf^\circ = 10.153 + 5.219\times10^{-3}T\ln T + 2.560\times10^{-6}T^2 + 10.500T^{-1} - 80.614\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = 7.970 - 14.825\times10^{-3}T - 0.322\times10^{-6}T^2 + 21.000T^{-1}$

$\Delta Gf^\circ = 7.970 + 14.825\times10^{-3}T\ln T + 0.322\times10^{-6}T^2 + 10.500T^{-1} - 131.337\times10^{-3}T$

458.4-1687 K: $\Delta Hf^\circ = -14.099 + 0.685\times10^{-3}T - 0.424\times10^{-6}T^2 - 1.950T^{-1}$

$\Delta Gf^\circ = -14.099 - 0.685\times10^{-3}T\ln T + 0.424\times10^{-6}T^2 - 0.975T^{-1} + 11.858\times10^{-3}T$

1687-2000 K: $\Delta Hf^\circ = -26.529 + 0.264\times10^{-3}T - 0.073\times10^{-6}T^2 + 96.550T^{-1}$

$\Delta Gf^\circ = -26.529 - 0.264\times10^{-3}T\ln T + 0.073\times10^{-6}T^2 + 48.275T^{-1} + 16.672\times10^{-3}T$

Source: Data are those estimated by Chase (24).

SiI_4(c,l,g)

Silicon Tetraiodide

[Formation: $Si(c,l) + 2I_2(c,l,g) = SiI_4(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	25.821	61.700	61.700	0	-45.300	-45.802	33.573
300	25.860	61.860	61.700	.048	-45.309	-45.805	33.368
386.8	27.677	68.653	62.523	2.371	-45.840	-45.886	25.926
386.8	27.677	68.653	62.523	2.371	-53.258	-45.886	25.926
393.65	27.820	69.140	62.634	2.561	-53.369	-45.755	25.402
393.65	39.135	81.080	62.634	7.261	-48.669	-45.755	25.402
400	39.198	81.706	62.931	7.510	-48.698	-45.707	24.973
458.4	39.774	87.086	65.673	9.816	-48.957	-45.246	21.572
458.4	39.774	87.086	65.673	9.816	-68.999	-45.246	21.572
500	40.185	90.559	67.601	11.479	-68.311	-43.118	18.846
575.8	40.933	96.283	71.009	14.553	-67.028	-39.394	14.952
575.8	25.283	115.811	71.009	25.797	-55.784	-39.394	14.952
600	25.333	116.854	72.837	26.410	-55.746	-38.706	14.098
700	25.462	120.770	79.413	28.950	-55.595	-35.879	11.202
800	25.547	124.176	84.800	31.501	-55.451	-33.069	9.034
900	25.606	127.188	89.345	34.059	-55.321	-30.279	7.353
1000	25.648	129.888	93.267	36.621	-55.197	-27.495	6.009
1100	25.680	132.335	96.710	39.188	-55.081	-24.740	4.915
1200	25.704	134.570	99.773	41.757	-54.974	-21.986	4.004
1300	25.723	136.628	102.529	44.329	-54.870	-19.240	3.234
1400	25.738	138.535	105.034	46.902	-54.778	-16.498	2.575
1500	25.750	140.311	107.327	49.476	-54.693	-13.781	2.008
1600	25.760	141.973	109.441	52.052	-54.613	-11.053	1.510
1687	25.768	143.337	111.154	54.293	-54.552	-8.666	1.123
1687	25.768	143.337	111.154	54.293	-66.634	-8.666	1.123
1700	25.769	143.535	111.401	54.628	-66.616	-8.216	1.056
1800	25.776	145.009	113.228	57.205	-66.483	-4.784	.581
1900	25.781	146.402	114.937	59.783	-66.353	-1.358	.156
2000	25.786	147.725	116.544	62.362	-66.224	2.054	-.224

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
393.65 K, melting point of SiI_4; $\Delta H°$ = 4.700 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
575.8 K, boiling point of SiI_4; $\Delta H°$ = 11.244 kcal/mol.
1687 K, melting point of Si; $\Delta H°$ = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-393.65 K: $Cp° = 25.820 + 2.862\times10^{-3}T$

$H°- H°_{298} = 25.820\times10^{-3}T + 1.431\times10^{-6}T^2 - 7.825$

393.65-575.8 K: $Cp° = 35.250 + 9.870\times10^{-3}T$

$H°- H°_{298} = 35.250\times10^{-3}T + 4.935\times10^{-6}T^2 - 7.380$

575.8-2000 K: $Cp° = 25.835 - 1.845\times10^{5}T^{-2}$

$H°- H°_{298} = 25.835\times10^{-3}T + 1.845\times10^{2}T^{-1} + 10.601$

SiI_4(c,l,g) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -43.127 - 5.613\times10^{-3}T - 1.904\times10^{-6}T^2 - 98.500T^{-1}$

$\Delta Gf^\circ = -43.127 + 5.613\times10^{-3}T\ln T + 1.904\times10^{-6}T^2 - 49.250T^{-1} - 40.967\times10^{-3}T$

386.8-393.65 K: $\Delta Hf^\circ = -46.037 - 18.421\times10^{-3}T + 1.080\times10^{-6}T^2 - 98.500T^{-1}$

$\Delta Gf^\circ = -46.037 + 18.421\times10^{-3}T\ln T - 1.080\times10^{-6}T^2 - 49.250T^{-1} - 108.598\times10^{-3}T$

393.65-458.4 K: $\Delta Hf^\circ = -45.592 - 8.991\times10^{-3}T + 4.584\times10^{-6}T^2 - 98.500T^{-1}$

$\Delta Gf^\circ = -45.592 + 8.991\times10^{-3}T\ln T - 4.584\times10^{-6}T^2 - 49.250T^{-1} - 52.000\times10^{-3}T$

458.4-575.8 K: $\Delta Hf^\circ = -75.019 + 11.689\times10^{-3}T + 4.448\times10^{-6}T^2 - 129.100T^{-1}$

$\Delta Gf^\circ = -75.019 - 11.689\times10^{-3}T\ln T - 4.448\times10^{-6}T^2 - 64.550T^{-1} + 138.926\times10^{-3}T$

575.8-1687 K: $\Delta Hf^\circ = -57.038 + 2.274\times10^{-3}T - 0.487\times10^{-6}T^2 + 55.400T^{-1}$

$\Delta Gf^\circ = -57.038 - 2.274\times10^{-3}T\ln T + 0.487\times10^{-6}T^2 + 27.700T^{-1} + 44.739\times10^{-3}T$

1687-2000 K: $\Delta Hf^\circ = -69.467 + 1.853\times10^{-3}T - 0.136\times10^{-6}T^2 + 153.900T^{-1}$

$\Delta Gf^\circ = -69.467 - 1.853\times10^{-3}T\ln T + 0.136\times10^{-6}T^2 + 76.950T^{-1} + 49.553\times10^{-3}T$

Sources: Data from Chase (24, 26).

$SiI_4(g)$

Silicon Tetraiodide (ideal gas)

[Formation: $Si(c,l) + 2I_2(c,l,g) = SiI_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	24.037	99.506	99.506	0	-26.400	-38.174	27.982
300	24.056	99.655	99.508	.044	-26.413	-38.247	27.863
386.8	24.671	105.855	100.261	2.164	-27.147	-41.583	23.495
386.8	24.671	105.855	100.261	2.164	-34.565	-41.583	23.495
400	24.764	106.684	100.459	2.490	-34.818	-41.818	22.848
458.4	24.975	110.077	101.473	3.944	-35.929	-42.757	20.385
458.4	24.975	110.077	101.473	3.944	-55.971	-42.757	20.385
500	25.126	112.253	102.281	4.986	-55.904	-41.558	18.165
600	25.333	116.854	104.337	7.510	-55.746	-38.706	14.098
700	25.462	120.770	106.413	10.050	-55.595	-35.879	11.202
800	25.547	124.176	108.425	12.601	-55.451	-33.069	9.034
900	25.606	127.188	110.345	15.159	-55.321	-30.279	7.353
1000	25.648	129.888	112.167	17.721	-55.197	-27.495	6.009
1100	25.680	132.335	113.891	20.288	-55.081	-24.740	4.915
1200	25.704	134.570	115.523	22.857	-54.974	-21.986	4.004
1300	25.723	136.628	117.067	25.429	-54.870	-19.240	3.234
1400	25.738	138.535	118.534	28.002	-54.778	-16.498	2.575
1500	25.750	140.311	119.927	30.576	-54.693	-13.781	2.008
1600	25.760	141.973	121.253	33.152	-54.613	-11.053	1.510
1687	25.768	143.337	122.357	35.393	-54.552	-8.666	1.123
1687	25.768	143.337	122.357	35.393	-66.634	-8.666	1.123
1700	25.769	143.535	122.519	35.728	-66.616	-8.216	1.056
1800	25.776	145.009	123.728	38.305	-66.483	-4.784	.581
1900	25.781	146.402	124.885	40.883	-66.353	-1.358	.156
2000	25.786	147.725	125.994	43.462	-66.224	2.054	-.224

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 25.692 + 0.088\times10^{-3}T - 1.494\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.692\times10^{-3}T + 0.044\times10^{-6}T^2 + 1.494\times10^{2}T^{-1} - 8.165$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -24.566 - 5.741\times10^{-3}T - 3.291\times10^{-6}T^2 + 50.900T^{-1}$

$\Delta Gf^\circ = -24.566 + 5.741\times10^{-3}T\ln T + 3.291\times10^{-6}T^2 + 25.450T^{-1} - 79.617\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -27.477 - 18.549\times10^{-3}T - 0.307\times10^{-6}T^2 + 50.900T^{-1}$

$\Delta Gf^\circ = -27.477 + 18.549\times10^{-3}T\ln T + 0.307\times10^{-6}T^2 + 25.450T^{-1} - 147.248\times10^{-3}T$

458.4-1687 K: $\Delta Hf^\circ = -56.903 + 2.131\times10^{-3}T - 0.443\times10^{-6}T^2 + 20.300T^{-1}$

$\Delta Gf^\circ = -56.903 - 2.131\times10^{-3}T\ln T + 0.443\times10^{-6}T^2 + 10.150T^{-1} + 43.678\times10^{-3}T$

1687-2000 K: $\Delta Hf^\circ = -69.332 + 1.710\times10^{-3}T - 0.092\times10^{-6}T^2 + 118.800T^{-1}$

$\Delta Gf^\circ = -69.332 - 1.710\times10^{-3}T\ln T + 0.092\times10^{-6}T^2 + 59.400T^{-1} + 48.492\times10^{-3}T$

Source: Data from Chase (24).

$SmCl_3(c,l)$
Samarium Trichloride
[Formation: $Sm(c) + 1.5Cl_2(g) = SmCl_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	23.790	35.880	35.880	0	-245.200	-227.107	166.472
300*	23.800	36.027	35.880	.044	-245.191	-226.996	165.364
400	25.100	43.064	36.832	2.493	-244.734	-221.000	120.747
500	25.900	48.750	38.664	5.043	-244.309	-215.112	94.024
600	26.600	53.538	40.755	7.670	-243.923	-209.314	76.241
700	27.300	57.696	42.885	10.368	-243.544	-203.571	63.557
800	28.000	61.390	44.971	13.135	-243.139	-197.889	54.060
900	28.700	64.727	46.984	15.969	-242.702	-192.258	46.686
950	29.000	66.285	47.959	17.410	-242.463	-189.461	43.585
950	34.000	77.864	47.959	28.410	-231.463	-189.461	43.585
1000	34.000	79.608	49.498	30.110	-230.973	-187.264	40.926
1100	34.000	82.849	52.385	33.510	-230.018	-182.948	36.348
1190	34.000	85.522	54.791	36.570	-229.194	-179.130	32.898
1190	34.000	85.522	54.791	36.570	-229.938	-179.130	32.898
1200	34.000	85.807	55.049	36.910	-229.845	-178.693	32.544
1300	34.000	88.528	57.520	40.310	-228.920	-174.477	29.332

*Data above 298 K estimated.

Phase changes: 950 K, melting point of $SmCl_3$; $\Delta H° = 11.000$ kcal/mol.
1190 K, α - β transition point of Sm; $\Delta H° = 0.744$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-950 K: $Cp° = 23.478 + 5.906\times10^{-3}T - 1.290\times10^{5}T^{-2}$

$H°- H°_{298} = 23.478\times10^{-3}T + 2.953\times10^{-6}T^2 + 1.290\times10^{2}T^{-1} - 7.695$

950-1300 K: $Cp° = 34.000$

$H°- H°_{298} = 34.000\times10^{-3}T - 3.890$

Formation equations (kcal/mol):

298.15-950 K: $\Delta Hf° = -245.412 + 2.038\times10^{-3}T + 1.336\times10^{-6}T^2 - 153.450T^{-1}$

$\Delta Gf° = -245.412 - 2.038\times10^{-3}T\ln T - 1.336\times10^{-6}T^2 - 76.725T^{-1} + 74.265\times10^{-3}T$

950-1190 K: $\Delta Hf° = -241.607 + 12.560\times10^{-3}T - 1.617\times10^{-6}T^2 - 282.450T^{-1}$

$\Delta Gf° = -241.607 - 12.560\times10^{-3}T\ln T + 1.617\times10^{-6}T^2 - 141.225T^{-1} + 139.669\times10^{-3}T$

1190-1300 K: $\Delta Hf° = -241.011 + 9.540\times10^{-3}T - 0.132\times10^{-6}T^2 - 102.450T^{-1}$

$\Delta Gf° = -241.011 - 9.540\times10^{-3}T\ln T + 0.132\times10^{-6}T^2 - 51.225T^{-1} + 119.486\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (207). Low-temperature heat capacities and entropy at 298 K from Sommers (220). High-temperature data estimated.

SmF_3(c,l)
Samarium Trifluoride
[Formation: $Sm(c,l) + 1.5F_2(g) = SmF_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	25.510	27.200	27.200	0	-398.900	-380.387	278.827
300	25.511	27.358	27.201	.047	-398.887	-380.273	277.025
400	25.568	34.705	28.203	2.601	-398.232	-374.170	204.435
500	25.621	40.416	30.094	5.161	-397.724	-368.213	160.944
600	25.674	45.092	32.215	7.726	-397.341	-362.352	131.985
700	25.727	49.054	34.345	10.296	-397.046	-356.541	111.316
763	25.760	51.272	35.653	11.917	-396.884	-352.903	101.082
763	32.198	51.884	35.653	12.384	-396.417	-352.903	101.082
800	30.383	53.364	36.439	13.540	-396.127	-350.800	95.833
900	27.666	56.759	38.515	16.420	-395.616	-345.167	83.817
1000	27.182	59.633	40.486	19.147	-395.280	-339.580	74.214
1100	28.157	62.260	42.346	21.905	-394.951	-334.033	66.365
1190	29.929	64.538	43.940	24.512	-394.568	-329.064	60.434
1190	29.929	64.538	43.940	24.512	-395.312	-329.064	60.434
1200	30.126	64.789	44.112	24.812	-395.257	-328.497	59.827
1300	32.794	67.301	45.799	27.953	-394.581	-322.968	54.295
1345	34.223	68.441	46.537	29.461	-394.185	-320.486	52.075
1345	34.223	68.441	46.537	29.461	-396.245	-320.486	52.075
1400	35.970	69.845	47.425	31.388	-395.721	-317.402	49.548
1500	39.523	72.446	49.006	35.160	-394.503	-311.845	45.435
1572	42.262	74.361	50.123	38.103	-393.403	-307.909	42.807
1572	35.597	82.346	50.123	50.653	-380.853	-307.909	42.807
1600	35.597	82.974	50.693	51.650	-380.573	-306.613	41.881
1700	35.597	85.132	52.656	55.209	-379.576	-302.016	38.826
1800	35.597	87.167	54.518	58.769	-378.583	-297.493	36.120
1900	35.597	89.092	56.287	62.329	-377.593	-293.013	33.704
2000	35.597	90.918	57.974	65.888	-376.609	-288.579	31.534

*Entropy and heat capacity at 298 K estimated.

Phase changes: 763 K, α - β transition point of SmF_3; $\Delta H°$ = 0.467 kcal/mol.
1190 K, α - β transition point of Sm; $\Delta H°$ = 0.744 kcal/mol.
1345 K, melting point of Sm; $\Delta H°$ = 2.060 kcal/mol.
1572 K, melting point of SmF_3; $\Delta H°$ = 12.550 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-763 K: $Cp° = 25.356 + 0.528\times10^{-3}T$
$H°- H°_{298} = 25.356\times10^{-3}T + 0.264\times10^{-6}T^2 - 7.583$

763-1572 K: $Cp° = -47.963 + 51.240\times10^{-3}T + 239.067\times10^{5}T^{-2}$
$H°- H°_{298} = -47.963\times10^{-3}T + 25.620\times10^{-6}T^2 - 239.067\times10^{2}T^{-1} + 65.397$

1572-2000 K: $Cp° = 35.597$
$H°- H°_{298} = 35.597\times10^{-3}T - 5.305$

SmF_3(c,l) - Continued

Formation equations (kcal/mol):

298.15-763 K: $\Delta Hf^\circ = -398.969 + 4.394\times10^{-3}T - 1.482\times10^{-6}T^2 - 330.750T^{-1}$

$\Delta Gf^\circ = -398.969 - 4.394\times10^{-3}T\ln T + 1.482\times10^{-6}T^2 - 165.375T^{-1} + 88.780\times10^{-3}T$

763-1190 K: $\Delta Hf^\circ = -325.988 - 68.925\times10^{-3}T + 23.874\times10^{-6}T^2 - 24237.450T^{-1}$

$\Delta Gf^\circ = -325.988 + 68.925\times10^{-3}T\ln T - 23.874\times10^{-6}T^2 - 12118.725T^{-1} - 453.628\times10^{-3}T$

1190-1345 K: $\Delta Hf^\circ = -325.393 - 71.945\times10^{-3}T + 25.359\times10^{-6}T^2 - 24057.450T^{-1}$

$\Delta Gf^\circ = -325.393 + 71.945\times10^{-3}T\ln T - 25.359\times10^{-6}T^2 - 12028.725T^{-1} - 473.811\times10^{-3}T$

1345-1572 K: $\Delta Hf^\circ = -326.404 - 72.725\times10^{-3}T + 25.359\times10^{-6}T^2 - 24057.450T^{-1}$

$\Delta Gf^\circ = -326.404 + 72.725\times10^{-3}T\ln T - 25.359\times10^{-6}T^2 - 12028.725T^{-1} - 478.679\times10^{-3}T$

1572-2000 K: $\Delta Hf^\circ = -397.106 + 10.835\times10^{-3}T - 0.261\times10^{-6}T^2 - 150.750T^{-1}$

$\Delta Gf^\circ = -397.106 - 10.835\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 - 75.375T^{-1} + 136.196\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Kim (123). Entropy and heat capacity at 298 K estimated. High-temperature data based on Spedding (222).

$SmF_3(g)$

Samarium Trifluoride (ideal gas)

[Formation: $Sm(c,l) + 1.5F_2(g) = SmF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	17.583	80.064	80.064	0	-296.600	-293.848	215.394
300	17.615	80.173	80.064	.033	-296.601	-293.832	214.054
400	19.016	85.447	80.774	1.869	-296.665	-292.899	160.031
500	19.926	89.795	82.155	3.820	-296.766	-291.943	127.607
600	20.526	93.485	83.745	5.844	-296.924	-290.970	105.984
700	20.933	96.681	85.370	7.918	-297.124	-289.958	90.528
800	21.218	99.496	86.962	10.027	-297.340	-288.919	78.928
900	21.421	102.008	88.498	12.159	-297.577	-287.852	69.899
1000	21.563	104.273	89.964	14.309	-297.818	-286.759	62.670
1100	21.660	106.333	91.360	16.470	-298.086	-285.648	56.752
1190	21.714	108.038	92.557	18.423	-298.357	-284.619	52.271
1190	21.714	108.038	92.557	18.423	-299.101	-284.619	52.271
1200	21.720	108.220	92.687	18.640	-299.130	-284.487	51.811
1300	21.750	109.960	93.950	20.813	-299.421	-283.265	47.620
1345	21.753	110.700	94.498	21.792	-299.554	-282.693	45.934
1345	21.753	110.700	94.498	21.792	-301.614	-282.693	45.934
1400	21.756	111.572	95.151	22.989	-301.820	-281.919	44.009
1500	21.741	113.073	96.297	25.164	-302.199	-280.482	40.866
1600	21.711	114.475	97.389	27.337	-302.586	-279.027	38.113
1700	21.670	115.790	98.434	29.506	-302.978	-277.537	35.679
1800	21.619	117.027	99.433	31.670	-303.383	-276.040	33.515
1900	21.563	118.195	100.390	33.829	-303.793	-274.508	31.575
2000	21.503	119.299	101.308	35.983	-304.215	-272.947	29.826

Phase changes: 1190 K, α - β transition point of Sm; $\Delta H° = 0.744$ kcal/mol.
1345 K, melting point of Sm; $\Delta H° = 2.060$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 21.348 + 0.344\times10^{-3}T - 3.438\times10^{5}T^{-2}$

$H°- H°_{298} = 21.348\times10^{-3}T + 0.172\times10^{-6}T^2 + 3.438\times10^{2}T^{-1} - 7.533$

Formation equations (kcal/mol):

298.15-1190 K: $\Delta Hf° = -296.619 + 0.386\times10^{-3}T - 1.574\times10^{-6}T^2 + 13.050T^{-1}$

$\Delta Gf° = -296.619 - 0.386\times10^{-3}T\ln T + 1.574\times10^{-6}T^2 + 6.525T^{-1} + 10.951\times10^{-3}T$

1190-1345 K: $\Delta Hf° = -296.023 - 2.634\times10^{-3}T - 0.089\times10^{-6}T^2 + 193.050T^{-1}$

$\Delta Gf° = -296.023 + 2.634\times10^{-3}T\ln T + 0.089\times10^{-6}T^2 + 96.525T^{-1} - 9.233\times10^{-3}T$

1345-2000 K: $\Delta Hf° = -297.034 - 3.414\times10^{-3}T - 0.089\times10^{-6}T^2 + 193.050T^{-1}$

$\Delta Gf° = -297.034 + 3.414\times10^{-3}T\ln T + 0.089\times10^{-6}T^2 + 96.525T^{-1} - 14.101\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Biefeld (15). Other data based on Myers (165) and Dieke (56).

$SnBr_2$(c,l)
Tin Dibromide
[Formation: $Sn(\beta,l) + Br_2(l,g) = SnBr_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	18.873	36.568	36.568	0	-58.200	-54.608	40.028
300*	18.890	36.685	36.568	.035	-58.210	-54.585	39.765
332.6	19.209	38.650	36.678	.656	-58.390	-54.183	35.603
332.6	19.209	38.650	36.678	.656	-65.455	-54.183	35.603
400	19.870	42.246	37.321	1.970	-65.184	-51.926	28.371
500	21.200	46.814	38.774	4.020	-64.727	-48.663	21.270
504	21.260	46.983	38.838	4.105	-64.707	-48.536	21.046
504	24.800	55.118	38.838	8.205	-60.607	-48.536	21.046
505.12	24.800	55.173	38.874	8.233	-60.598	-48.509	20.988
505.12	24.800	55.173	38.874	8.233	-62.278	-48.509	20.988
600	24.800	59.442	41.799	10.586	-61.423	-45.993	16.753
700	24.800	63.265	44.599	13.066	-60.520	-43.493	13.579
800	24.800	66.577	47.145	15.546	-59.615	-41.122	11.234
900	24.800	69.498	49.469	18.026	-58.714	-38.865	9.438
1000	24.800	72.111	51.605	20.506	-57.814	-36.709	8.023

*Data above 298 K except temperature and enthalpy of fusion estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
504 K, melting point of $SnBr_2$; ΔH° = 4.100 kcal/mol.
505.12 K, melting point of Sn; ΔH° = 1.680 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-504 K: $Cp^\circ = 13.301 + 14.884\times10^{-3}T + 1.008\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.301\times10^{-3}T + 7.442\times10^{-6}T^2 - 1.008\times10^{2}T^{-1} - 4.289$

504-1000 K: $Cp^\circ = 24.800$

$H^\circ - H^\circ_{298} = 24.800\times10^{-3}T - 4.294$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -55.440 - 9.758\times10^{-3}T + 5.200\times10^{-6}T^2 - 93.200T^{-1}$

$\Delta Gf^\circ = -55.440 + 9.758\times10^{-3}T\ln T - 5.200\times10^{-6}T^2 - 46.600T^{-1} - 50.732\times10^{-3}T$

332.6-504 K: $\Delta Hf^\circ = -65.441 - 0.597\times10^{-3}T + 5.045\times10^{-6}T^2 - 124.600T^{-1}$

$\Delta Gf^\circ = -65.441 + 0.597\times10^{-3}T\ln T - 5.045\times10^{-6}T^2 - 62.300T^{-1} + 32.623\times10^{-3}T$

504-505.12 K: $\Delta Hf^\circ = -65.446 + 10.902\times10^{-3}T - 2.397\times10^{-6}T^2 - 23.800T^{-1}$

$\Delta Gf^\circ = -65.446 - 10.902\times10^{-3}T\ln T + 2.397\times10^{-6}T^2 - 11.900T^{-1} + 100.238\times10^{-3}T$

505.12-1000 K: $\Delta Hf^\circ = -67.411 + 9.679\times10^{-3}T - 0.236\times10^{-6}T^2 + 154.000T^{-1}$

$\Delta Gf^\circ = -67.411 - 9.679\times10^{-3}T\ln T + 0.236\times10^{-6}T^2 + 77.000T^{-1} + 97.259\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Low-temperature heat capacities and entropy at 298 K from Berezovskii (11). Temperature and enthalpy of fusion from Sevast'yanova (208). Other high-temperature data derived from estimated heat capacities.

$SnBr_4$ (g)

Tin Tetrabromide (ideal gas)

[Formation: $Sn(\beta,l) + 2Br_2(l,g) = SnBr_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	24.710	98.620	98.620	0	-75.200	-79,263	58.100
300	24.730	98.770	98.620	.045	-75.233	-79.287	57.760
332.6	24.877	101.329	98.762	.854	-75.813	-79.698	52.368
332.6	24.877	101.329	98.762	.854	-89.943	-79.698	52.368
400	25.180	105.960	99.597	2.545	-89.884	-77.633	42.416
500	25.420	111.600	101.450	5.075	-89.829	-74.576	32.597
505.12	25.427	111.859	101.554	5.205	-89.828	-74.421	32.199
505.12	25.427	111.859	101.554	5.205	-91.508	-74.421	32.199
600	25.550	116.250	103.542	7.625	-91.429	-71.214	25.939
700	25.620	120.190	105.647	10.180	-91.344	-67.853	21.184
800	25.670	123.620	107.689	12.745	-91.249	-64.506	17.622
900	25.700	126.640	109.623	15.315	-91.157	-61.164	14.852
1000	25.730	129.350	111.465	17.885	-91.067	-57.839	12.641

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
505.12 K, melting point of Sn; ΔH° = 1.680 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $C_p^\circ = 25.698 + 0.152\times10^{-3}T - 0.919\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.698\times10^{-3}T + 0.076\times10^{-6}T^2 + 0.919\times10^{2}T^{-1} - 7.977$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -70.743 - 15.452\times10^{-3}T - 2.066\times10^{-6}T^2 + 99.500T^{-1}$

$\Delta Gf^\circ = -70.743 + 15.452\times10^{-3}T\ln T + 2.066\times10^{-6}T^2 + 49.750T^{-1} - 117.790\times10^{-3}T$

332.6-505.12 K: $\Delta Hf^\circ = -90.744 + 2.870\times10^{-3}T - 2.376\times10^{-6}T^2 + 36.700T^{-1}$

$\Delta Gf^\circ = -90.744 - 2.870\times10^{-3}T\ln T + 2.376\times10^{-6}T^2 + 18.350T^{-1} + 48.921\times10^{-3}T$

505.12-1000 K: $\Delta Hf^\circ = -92.709 + 1.647\times10^{-3}T - 0.215\times10^{-6}T^2 + 214.500T^{-1}$

$\Delta Gf^\circ = -92.709 - 1.647\times10^{-3}T\ln T + 0.215\times10^{-6}T^2 + 107.250T^{-1} + 45.942\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Other data from Ananthanarayanan (4).

SnCl(g)
Tin Monochloride (ideal gas)
[Formation: $Sn(\beta,l) + 0.5Cl_2(g) = SnCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.565	60.540	60.540	0	8.284	1.826	-1.339
300	8.570	60.593	60.540	.016	8.281	1.786	-1.301
400	8.771	63.088	60.881	.883	8.066	-.347	.190
500	8.938	65.063	61.525	1.769	7.814	-2.421	1.058
505.12	8.947	65.154	61.561	1.815	7.800	-2.527	1.093
505.12	8.947	65.154	61.561	1.815	6.120	-2.527	1.093
600	9.114	66.708	62.256	2.671	5.908	-4.129	1.504
700	9.294	68.127	62.996	3.592	5.706	-5.785	1.806
800	9.464	69.379	63.716	4.530	5.521	-7.414	2.025
900	9.611	70.503	64.410	5.484	5.350	-9.020	2.190
1000	9.730	71.522	65.071	6.451	5.190	-10.610	2.319
1100	9.821	72.454	65.700	7.429	5.039	-12.182	2.420
1200	9.885	73.311	66.299	8.414	4.894	-13.741	2.503
1300	9.928	74.104	66.869	9.405	4.754	-15.288	2.570
1400	9.954	74.841	67.412	10.400	4.617	-16.823	2.626
1500	9.966	75.528	67.931	11.396	4.480	-18.349	2.673
1600	9.968	76.171	68.426	12.392	4.342	-19.868	2.714
1700	9.963	76.776	68.900	13.389	4.205	-21.378	2.748
1800	9.953	77.345	69.353	14.385	4.065	-22.878	2.778
1900	9.941	77.883	69.788	15.380	3.924	-24.370	2.803
2000	9.927	78.392	70.205	16.373	3.779	-25.856	2.825

Phase change: 505.12 K, melting point of Sn; ΔH° = 1.680 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.954 + 0.674\times10^{-3}T - 0.524\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.954\times10^{-3}T + 0.337\times10^{-6}T^2 + 0.524\times10^{2}T^{-1} - 2.875$

Formation equations (kcal/mol):

298.15-505.12 K: $\Delta Hf^\circ = 8.507 - 0.427\times10^{-3}T - 2.049\times10^{-6}T^2 + 25.850T^{-1}$

$\Delta Gf^\circ = 8.507 + 0.427\times10^{-3}T\ln T + 2.049\times10^{-6}T^2 + 12.925T^{-1} - 25.599\times10^{-3}T$

505.12-2000 K: $\Delta Hf^\circ = 6.541 - 1.650\times10^{-3}T + 0.112\times10^{-6}T^2 + 203.650T^{-1}$

$\Delta Gf^\circ = 6.541 + 1.650\times10^{-3}T\ln T - 0.112\times10^{-6}T^2 + 101.825T^{-1} - 28.577\times10^{-3}T$

Source: Data from Gurvich (94).

$SnCl_2(c,l,g)$
Tin Dichloride
[Formation: $Sn(\beta,l) + Cl_2(g) = SnCl_2(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	18.654	32.051	32.051	0	-78.400	-68.419	50.152
300*	18.670	32.166	32.051	.035	-78.392	-68.357	49.797
400	19.710	37.681	32.793	1.955	-77.969	-65.074	35.554
500	20.850	42.198	34.238	3.980	-77.508	-61.903	27.058
505.12	20.914	42.411	34.320	4.087	-77.483	-61.745	26.715
505.12	20.914	42.411	34.320	4.087	-79.163	-61.745	26.715
520	21.100	43.021	34.560	4.400	-79.084	-61.233	25.735
520	24.000	49.752	34.560	7.900	-75.584	-61.233	25.735
600	24.000	53.186	36.819	9.820	-74.911	-59.070	21.516
700	24.000	56.886	39.429	12.220	-74.073	-56.497	17.639
800	24.000	60.091	41.816	14.620	-73.239	-54.044	14.764
886	24.000	62.543	43.706	16.690	-72.519	-52.013	12.830
886	13.802	87.826	43.706	39.090	-50.119	-52.013	12.830
900	13.806	88.042	44.396	39.281	-50.148	-52.044	12.638
1000	13.826	89.498	48.836	40.662	-50.341	-52.247	11.418
1100	13.840	90.816	52.592	42.046	-50.534	-52.427	10.416
1200	13.851	92.021	55.829	43.430	-50.730	-52.591	9.578
1300	13.860	93.130	58.656	44.816	-50.926	-52.738	8.866
1400	13.867	94.158	61.157	46.202	-51.124	-52.870	8.253
1500	13.872	95.115	63.389	47.589	-51.323	-52.988	7.720
1600	13.877	96.010	65.399	48.977	-51.523	-53.093	7.252
1700	13.881	96.851	67.225	50.364	-51.725	-53.184	6.837
1800	13.884	97.645	68.893	51.753	-51.927	-53.264	6.467
1900	13.887	98.396	70.427	53.141	-52.131	-53.332	6.134
2000	13.889	99.108	71.843	54.530	-52.337	-53.391	5.834

*Heat capacities for $SnCl_2(c,l)$ above 298 K estimated.

Phase changes: 505.12 K, melting point of Sn; ΔH° = 1.680 kcal/mol.
520 K, melting point of $SnCl_2$; ΔH° = 3.500 kcal/mol.
886 K, boiling point of $SnCl_2$; ΔH° = 22.400 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-520 K: $Cp^\circ = 15.467 + 10.662\times10^{-3}T + 0.007\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 15.467\times10^{-3}T + 5.331\times10^{-6}T^2 - 0.007\times10^{2}T^{-1} - 5.083$

520-886 K: $Cp^\circ = 24.017$

$H^\circ - H^\circ_{298} = 24.017\times10^{-3}T - 4.589$

886-2000 K: $Cp^\circ = 13.758 + 0.080\times10^{-3}T - 0.214\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.758\times10^{-3}T + 0.040\times10^{-6}T^2 + 0.214\times10^{2}T^{-1} + 26.845$

$SnCl_2$(c,l,g) - Continued

Formation equations (kcal/mol):

298.15-505.12 K: $\Delta Hf^\circ = -78.950 + 1.672\times10^{-3}T + 2.901\times10^{-6}T^2 - 61.400T^{-1}$

$\Delta Gf^\circ = -78.950 - 1.672\times10^{-3}T\ln T - 2.901\times10^{-6}T^2 - 30.700T^{-1} + 46.058\times10^{-3}T$

505.12-520 K: $\Delta Hf^\circ = -80.916 + 0.449\times10^{-3}T + 5.062\times10^{-6}T^2 + 116.400T^{-1}$

$\Delta Gf^\circ = -80.916 - 0.449\times10^{-3}T\ln T - 5.062\times10^{-6}T^2 + 58.200T^{-1} + 43.079\times10^{-3}T$

520-886 K: $\Delta Hf^\circ = -80.422 + 8.999\times10^{-3}T - 0.269\times10^{-6}T^2 + 117.100T^{-1}$

$\Delta Gf^\circ = -80.422 - 8.999\times10^{-3}T\ln T + 0.269\times10^{-6}T^2 + 58.550T^{-1} + 92.826\times10^{-3}T$

886-2000 K: $\Delta Hf^\circ = -48.988 - 1.260\times10^{-3}T - 0.229\times10^{-6}T^2 + 138.500T^{-1}$

$\Delta Gf^\circ = -48.988 + 1.260\times10^{-3}T\ln T + 0.229\times10^{-6}T^2 + 69.250T^{-1} - 12.256\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Vasil'ev (249). Low-temperature heat capacities and entropy at 298 K from Paukov (192). High-temperature data for crystal and liquid derived from estimated heat capacities. Temperature and enthalpy of fusion from Sevast'yanova (208). Data for gas from Gurvich (94).

$SnCl_2(g)$

Tin Dichloride (ideal gas)

[Formation: $Sn(\beta,l) + Cl_2(g) = SnCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	13.058	73.075	73.075	0	-47.310	-49.561	36.329
300	13.067	73.156	73.076	.024	-47.313	-49.575	36.115
400	13.410	76.968	73.593	1.350	-47.484	-50.304	27.484
500	13.582	79.981	74.579	2.701	-47.697	-50.984	22.285
505.12	13.587	80.119	74.634	2.771	-47.710	-51.019	22.074
505.12	13.587	80.119	74.634	2.771	-49.390	-51.019	22.074
600	13.679	82.467	75.694	4.064	-49.577	-51.305	18.688
700	13.739	84.581	76.817	5.435	-49.768	-51.578	16.103
800	13.778	86.418	77.904	6.811	-49.958	-51.824	14.158
900	13.806	88.042	78.941	8.191	-50.148	-52.044	12.638
1000	13.826	89.498	79.926	9.572	-50.341	-52.247	11.418
1100	13.840	90.816	80.856	10.956	-50.534	-52.427	10.416
1200	13.851	92.021	81.738	12.340	-50.730	-52.591	9.578
1300	13.860	93.130	82.572	13.726	-50.926	-52.738	8.866
1400	13.867	94.158	83.364	15.112	-51.124	-52.870	8.253
1500	13.872	95.115	84.116	16.499	-51.323	-52.988	7.720
1600	13.877	96.010	84.831	17.887	-51.523	-53.093	7.252
1700	13.881	96.851	85.513	19.274	-51.725	-53.184	6.837
1800	13.884	97.645	86.166	20.663	-51.927	-53.264	6.467
1900	13.887	98.396	86.790	22.051	-52.131	-53.332	6.134
2000	13.889	99.108	87.388	23.440	-52.337	-53.391	5.834

Phase change: 505.12 K, melting point of Sn; ΔH° = 1.680 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.859 + 0.032\times10^{-3}T - 0.721\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.859\times10^{-3}T + 0.016\times10^{-6}T^2 + 0.721\times10^{2}T^{-1} - 4.375$

Formation equations (kcal/mol):

298.15-505.12 K: $\Delta Hf^\circ = -47.153 + 0.064\times10^{-3}T - 2.414\times10^{-6}T^2 + 11.400T^{-1}$

$\Delta Gf^\circ = -47.153 - 0.064\times10^{-3}T\ln T + 2.414\times10^{-6}T^2 + 5.700T^{-1} - 8.496\times10^{-3}T$

505.12-2000 K: $\Delta Hf^\circ = -49.118 - 1.159\times10^{-3}T - 0.253\times10^{-6}T^2 + 189.200T^{-1}$

$\Delta Gf^\circ = -49.118 + 1.159\times10^{-3}T\ln T + 0.253\times10^{-6}T^2 + 94.600T^{-1} - 11.474\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on George (88). Other data from Gurvich (94).

$SnCl_4(l,g)$
Tin Tetrachloride
[Formation: $Sn(\beta,l) + 2Cl_2(g) = SnCl_4(l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	39.500	61.840	61.840	0	-122.200	-105.213	77.122
300	39.600	62.090	61.857	.070	-122.172	-105.112	76.573
382	44.660	72.220	63.007	3.520	-120.623	-100.632	57.573
382	24.340	93.140	63.007	11.510	-112.633	-100.632	57.573
400	24.460	94.260	64.385	11.950	-112.619	-100.065	54.672
500	24.930	99.780	70.940	14.420	-112.566	-96.938	42.371
505.12	24.944	100.034	71.234	14.548	-112.565	-96.779	41.873
505.12	24.944	100.034	71.234	14.548	-114.245	-96.779	41.873
600	25.200	104.350	76.133	16.930	-114.168	-93.498	34.056
700	25.360	108.240	80.440	19.460	-114.078	-90.053	28.116
800	25.470	111.640	84.140	22.000	-113.990	-86.636	23.667
900	25.540	114.640	87.362	24.550	-113.900	-83.217	20.208
1000	25.600	117.340	90.230	27.110	-113.808	-79.818	17.444

*Data extrapolated 294 to 382 K.

Phase changes: 240 K, melting point of $SnCl_4$; $\Delta H°$ = 2.190 kcal/mol.
382 K, boiling point of $SnCl_4$; $\Delta H°$ = 7.990 kcal/mol.
505.12 K, melting point of Sn; $\Delta H°$ = 1.680 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-382 K: $Cp° = 21.866 + 59.146\times10^{-3}T$
$H°- H°_{298} = 21.866\times10^{-3}T + 29.573\times10^{-6}T^2 - 9.148$

382-1000 K: $Cp° = 25.699 + 0.114\times10^{-3}T - 2.048\times10^{5}T^{-2}$
$H°- H°_{298} = 25.699\times10^{-3}T + 0.057\times10^{-6}T^2 + 2.048\times10^{2}T^{-1} + 1.149$

Formation equations (kcal/mol):

298.15-382 K: $\Delta Hf° = -123.947 - 0.756\times10^{-3}T + 27.055\times10^{-6}T^2 - 129.000T^{-1}$
$\Delta Gf° = -123.947 + 0.756\times10^{-3}T\ln T - 27.055\times10^{-6}T^2 - 64.500T^{-1} + 67.320\times10^{-3}T$

382-505.12 K: $\Delta Hf° = -113.650 + 3.077\times10^{-3}T - 2.461\times10^{-6}T^2 + 75.800T^{-1}$
$\Delta Gf° = -113.650 - 3.077\times10^{-3}T\ln T + 2.461\times10^{-6}T^2 + 37.900T^{-1} + 51.177\times10^{-3}T$

505.12-1000 K: $\Delta Hf° = -115.616 + 1.854\times10^{-3}T - 0.300\times10^{-6}T^2 + 253.600T^{-1}$
$\Delta Gf° = -115.616 - 1.854\times10^{-3}T\ln T + 0.300\times10^{-6}T^2 + 126.800T^{-1} + 48.199\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Low-temperature heat capacities, entropy at 298 K, and fusion data from Latimer (140). Data extrapolated 294 to 382 K. Data for gas from Ananthanarayanan (4). Boiling data from Kabesh (113).

$SnCl_4$(g)
Tin Tetrachloride (ideal gas)
[Formation: $Sn(\beta,l) + 2Cl_2(g) = SnCl_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	23.530	87.200	87.200	0	-112.700	-103.274	75.701
300	23.560	87.350	87.200	.045	-112.697	-103.215	75.191
400	24.460	94.260	88.135	2.450	-112.619	-100.065	54.672
500	24.930	99.780	89.940	4.920	-112.566	-96.938	42.371
505.12	24.944	100.034	90.041	5.048	-112.565	-96.779	41.873
505.12	24.944	100.034	90.041	5.048	-114.245	-96.779	41.873
600	25.200	104.350	91.967	7.430	-114.168	-93.498	34.056
700	25.360	108.240	94.011	9.960	-114.078	-90.053	28.116
800	25.470	111.640	96.015	12.500	-113.990	-86.636	23.667
900	25.540	114.640	97.918	15.050	-113.900	-83.217	20.208
1000	25.600	117.340	99.730	17.610	-113.808	-79.818	17.444

Phase change: 505.12 K, melting point of Sn; $\Delta H° = 1.680$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 25.485 + 0.338\times10^{-3}T - 1.827\times10^{5}T^{-2}$

$H°- H°_{298} = 25.485\times10^{-3}T + 0.169\times10^{-6}T^{2} + 1.827\times10^{2}T^{-1} - 8.226$

Formation equations (kcal/mol):

298.15-505.12 K: $\Delta Hf° = -113.525 + 2.863\times10^{-3}T - 2.349\times10^{-6}T^{2} + 53.700T^{-1}$

$\Delta Gf° = -113.525 - 2.863\times10^{-3}T\ln T + 2.349\times10^{-6}T^{2} + 26.850T^{-1} + 49.693\times10^{-3}T$

505.12-1000 K: $\Delta Hf° = -115.491 + 1.640\times10^{-3}T - 0.188\times10^{-6}T^{2} + 231.500T^{-1}$

$\Delta Gf° = -115.491 - 1.640\times10^{-3}T\ln T + 0.188\times10^{-6}T^{2} + 115.750T^{-1} + 46.714\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Other data from Ananthanarayanan (4).

SnF(g)

Tin Monofluoride (ideal gas)

[Formation: $Sn(\beta,l) + 0.5F_2(g) = SnF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.055	57.721	57.721	0	-22.710	-29.050	21.294
300	8.064	57.771	57.721	.015	-22.714	-29.089	21.191
400	8.421	60.143	58.043	.840	-22.940	-31.180	17.036
500	8.694	62.052	58.660	1.696	-23.198	-33.211	14.516
505.12	8.707	62.141	58.695	1.741	-23.212	-33.315	14.414
505.12	8.707	62.141	58.695	1.741	-24.892	-33.315	14.414
600	8.939	63.659	59.362	2.578	-25.104	-34.874	12.703
700	9.165	65.055	60.078	3.484	-25.306	-36.485	11.391
800	9.364	66.292	60.779	4.410	-25.491	-38.071	10.400
900	9.529	67.404	61.454	5.355	-25.662	-39.631	9.624
1000	9.660	68.416	62.101	6.315	-25.822	-41.176	8.999
1100	9.757	69.341	62.717	7.286	-25.974	-42.704	8.484
1200	9.825	70.193	63.306	8.265	-26.120	-44.218	8.053
1300	9.870	70.981	63.866	9.250	-26.263	-45.720	7.686
1400	9.896	71.714	64.400	10.239	-26.404	-47.211	7.370
1500	9.907	72.397	64.911	11.229	-26.545	-48.692	7.094
1600	9.908	73.037	65.400	12.220	-26.688	-50.166	6.852
1700	9.902	73.637	65.866	13.210	-26.832	-51.629	6.637
1800	9.891	74.203	66.314	14.200	-26.978	-53.083	6.445
1900	9.877	74.737	66.743	15.189	-27.125	-54.527	6.272
2000	9.862	75.244	67.157	16.175	-27.278	-55.970	6.116

Phase change: 505.12 K, melting point of Sn; $\Delta H° = 1.680$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.778 + 0.778\times10^{-3}T - 0.849\times10^{5}T^{-2}$

$H°- H°_{298} = 8.778\times10^{-3}T + 0.389\times10^{-6}T^{2} + 0.849\times10^{2}T^{-1} - 2.936$

Formation equations (kcal/mol):

298.15-505.12 K: $\Delta Hf° = -22.538 - 0.444\times10^{-3}T - 2.040\times10^{-6}T^{2} + 42.250T^{-1}$

$\Delta Gf° = -22.538 + 0.444\times10^{-3}T\ln T + 2.040\times10^{-6}T^{2} + 21.125T^{-1} - 25.216\times10^{-3}T$

505.12-2000 K: $\Delta Hf° = -24.504 - 1.667\times10^{-3}T + 0.121\times10^{-6}T^{2} + 220.050T^{-1}$

$\Delta Gf° = -24.504 + 1.667\times10^{-3}T\ln T - 0.121\times10^{-6}T^{2} + 110.025T^{-1} - 28.194\times10^{-3}T$

Source: Data from Gurvich (94).

$SnF_2(c,l)$
Tin Difluoride
[Formation: $Sn(\beta,l) + F_2(g) = SnF_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	17.303	22.992	22.992	0	-155.000	-143.764	105.380
300	17.329	23.099	22.992	.032	-154.994	-143.694	104.680
400	18.750	28.279	23.689	1.836	-154.626	-139.980	76.481
488.2	20.003	32.136	24.874	3.545	-154.250	-136.789	61.235
488.2	23.900	37.277	24.874	6.055	-151.740	-136.789	61.235
500	23.900	37.848	25.174	6.337	-151.640	-136.428	59.632
505.12	23.900	38.091	25.304	6.459	-151.598	-136.274	58.961
505.12	23.900	38.091	25.304	6.459	-153.278	-136.274	58.961
600	23.900	42.205	27.660	8.727	-152.454	-133.150	48.499
700	23.900	45.889	30.008	11.117	-151.596	-130.000	40.587
800	23.900	49.081	32.197	13.507	-150.748	-126.974	34.687
900	23.900	51.896	34.233	15.897	-149.909	-124.051	30.123
1000	23.900	54.414	36.127	18.287	-149.079	-121.224	26.493

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 488.2 K, melting point of SnF_2; ΔH° = 2.510 kcal/mol.
505.12 K, melting point of Sn; ΔH° = 1.680 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-488.2 K: $Cp^\circ = 13.069 + 14.204\times10^{-3}T - 0.001\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 13.069\times10^{-3}T + 7.102\times10^{-6}T^2 + 0.001\times10^{2}T^{-1} - 4.528$

488.2-1000 K: $Cp^\circ = 23.900$
$H^\circ - H^\circ_{298} = 23.900\times10^{-3}T - 5.613$

Formation equations (kcal/mol):

298.15-488.2 K: $\Delta Hf^\circ = -154.975 - 0.407\times10^{-3}T + 4.586\times10^{-6}T^2 - 92.800T^{-1}$
$\Delta Gf^\circ = -154.975 + 0.407\times10^{-3}T\ln T - 4.586\times10^{-6}T^2 - 46.400T^{-1} + 37.174\times10^{-3}T$

488.2-505.12 K: $\Delta Hf^\circ = -156.060 + 10.424\times10^{-3}T - 2.516\times10^{-6}T^2 - 92.900T^{-1}$
$\Delta Gf^\circ = -156.060 - 10.424\times10^{-3}T\ln T + 2.516\times10^{-6}T^2 - 46.450T^{-1} + 102.981\times10^{-3}T$

505.12-1000 K: $\Delta Hf^\circ = -158.025 + 9.201\times10^{-3}T - 0.355\times10^{-6}T^2 + 84.900T^{-1}$
$\Delta Gf^\circ = -158.025 - 9.201\times10^{-3}T\ln T + 0.355\times10^{-6}T^2 + 42.450T^{-1} + 100.002\times10^{-3}T$

Sources: Data from Gurvich (94) who estimated all except enthalpy of formation at 298 K.

$SnF_2(g)$
Tin Difluoride (ideal gas)
[Formation: $Sn(\beta,l) + F_2(g) = SnF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	11.874	67.403	67.403	0	-115.668	-117.673	86.255
300	11.891	67.476	67.403	.022	-115.672	-117.685	85.733
400	12.603	71.004	67.879	1.250	-115.880	-118.324	64.648
500	13.013	73.864	68.798	2.533	-116.112	-118.908	51.974
505.12	13.026	73.997	68.850	2.600	-116.125	-118.938	51.460
505.12	13.026	73.997	68.850	2.600	-117.805	-118.938	51.460
600	13.262	76.261	69.849	3.847	-118.002	-119.131	43.393
700	13.422	78.318	70.915	5.182	-118.199	-119.303	37.248
800	13.530	80.118	71.955	6.530	-118.393	-119.448	32.631
900	13.607	81.716	72.953	7.887	-118.587	-119.567	29.034
1000	13.663	83.153	73.902	9.251	-118.783	-119.667	26.153
1100	13.704	84.457	74.803	10.619	-118.981	-119.745	23.791
1200	13.736	85.651	75.659	11.991	-119.180	-119.806	21.819
1300	13.762	86.751	76.469	13.366	-119.380	-119.849	20.148
1400	13.782	87.772	77.241	14.743	-119.583	-119.878	18.714
1500	13.798	88.723	77.975	16.122	-119.787	-119.892	17.468
1600	13.811	89.614	78.675	17.503	-119.992	-119.893	16.376
1700	13.823	90.452	79.343	18.885	-120.198	-119.880	15.411
1800	13.832	91.242	79.983	20.267	-120.408	-119.855	14.552
1900	13.840	91.990	80.595	21.651	-120.617	-119.817	13.782
2000	13.847	92.700	81.182	23.035	-120.830	-119.772	13.088

Phase change: 505.12 K, melting point of Sn; $\Delta H° = 1.680$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.584 + 0.190\times10^{-3}T - 1.570\times10^{5}T^{-2}$

$H°- H°_{298} = 13.584\times10^{-3}T + 0.095\times10^{-6}T^2 + 1.570\times10^{2}T^{-1} - 4.585$

Formation equations (kcal/mol):

298.15-505.12 K: $\Delta Hf° = -115.700 + 0.108\times10^{-3}T - 2.421\times10^{-6}T^2 + 64.100T^{-1}$

$\Delta Gf° = -115.700 - 0.108\times10^{-3}T\ln T + 2.421\times10^{-6}T^2 + 32.050T^{-1} - 7.084\times10^{-3}T$

505.12-2000 K: $\Delta Hf° = -117.666 - 1.115\times10^{-3}T - 0.260\times10^{-6}T^2 + 241.900T^{-1}$

$\Delta Gf° = -117.666 + 1.115\times10^{-3}T\ln T + 0.260\times10^{-6}T^2 + 120.950T^{-1} - 10.062\times10^{-3}T$

Source: Data from Gurvich (94).

SnI_2(c,l)
Tin Diiodide
[Formation: $Sn(\beta,l) + I_2(c,l,g) = SnI_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.750	40.270	40.270	0	-34.390	-34.472	25.269
300*	18.760	40.386	40.270	.035	-34.391	-34.472	25.113
386.8	19.446	45.239	40.863	1.693	-34.518	-34.483	19.483
386.8	19.446	45.239	40.863	1.693	-38.227	-34.483	19.483
400	19.550	45.893	41.018	1.950	-38.315	-34.354	18.770
458.4	20.006	48.586	41.810	3.106	-38.694	-33.745	16.088
458.4	20.006	48.586	41.810	3.106	-48.715	-33.745	16.088
500	20.330	50.338	42.448	3.945	-48.549	-32.392	14.159
505.12	20.372	50.545	42.529	4.049	-48.529	-32.228	13.944
505.12	20.372	50.545	42.529	4.049	-50.209	-32.228	13.944
593	21.100	53.869	43.970	5.870	-49.784	-29.132	10.736
593	23.900	61.120	43.970	10.170	-45.484	-29.132	10.736
600	23.900	61.400	44.172	10.337	-45.428	-28.939	10.541
700	23.900	65.084	46.903	12.727	-44.621	-26.254	8.197
800	23.900	68.276	49.380	15.117	-43.812	-23.686	6.471
900	23.900	71.091	51.639	17.507	-43.006	-21.219	5.153
1000	23.900	73.609	53.712	19.897	-42.201	-18.841	4.118

*Heat capacities above 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
505.12 K, melting point of Sn; $\Delta H°$ = 1.680 kcal/mol.
593 K, melting point of SnI_2; $\Delta H°$ = 4.300 kcal/mol.
980 K, boiling point of SnI_2; $\Delta H°$ at 298 K = 30.76 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-593 K: $Cp° = 16.302 + 8.034\times10^{-3}T + 0.047\times10^{5}T^{-2}$
$H°- H°_{298} = 16.302\times10^{-3}T + 4.017\times10^{-6}T^2 - 0.047\times10^{2}T^{-1} - 5.202$
593-1000 K: $Cp° = 23.900$
$H°- H°_{298} = 23.900\times10^{-3}T - 4.003$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -33.956 - 1.543\times10^{-3}T + 0.183\times10^{-6}T^2 + 2.900T^{-1}$
$\Delta Gf° = -33.956 + 1.543\times10^{-3}T\ln T - 0.183\times10^{-6}T^2 + 1.450T^{-1} - 10.485\times10^{-3}T$
386.8-458.4 K: $\Delta Hf° = -35.411 - 7.947\times10^{-3}T + 1.675\times10^{-6}T^2 + 2.900T^{-1}$
$\Delta Gf° = -35.411 + 7.947\times10^{-3}T\ln T - 1.675\times10^{-6}T^2 + 1.450T^{-1} - 44.300\times10^{-3}T$
458.4-505.12 K: $\Delta Hf° = -50.124 + 2.393\times10^{-3}T + 1.607\times10^{-6}T^2 - 12.400T^{-1}$
$\Delta Gf° = -50.124 - 2.393\times10^{-3}T\ln T - 1.607\times10^{-6}T^2 - 6.200T^{-1} + 51.163\times10^{-3}T$
505.12-593 K: $\Delta Hf° = -52.090 + 1.170\times10^{-3}T + 3.768\times10^{-6}T^2 + 165.400T^{-1}$
$\Delta Gf° = -52.090 - 1.170\times10^{-3}T\ln T - 3.768\times10^{-6}T^2 + 82.700T^{-1} + 48.184\times10^{-3}T$
593-1000 K: $\Delta Hf° = -50.891 + 8.768\times10^{-3}T - 0.249\times10^{-6}T^2 + 170.100T^{-1}$
$\Delta Gf° = -50.891 - 8.768\times10^{-3}T\ln T + 0.249\times10^{-6}T^2 + 85.050T^{-1} + 92.288\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Cartwright (21). Low-temperature heat capacities and entropy at 298 K from Anisimov (7). High-temperature data based on estimated heat capacities. Fusion data from Sevast'yanova (208). Boiling temperature and enthalpy of vaporization at 298 K from Zhamskaya (270).

$SnI_4(c,l,g)$

Tin Tetraiodide

[Formation: $Sn(\beta,l) + 2I_2(c,l,g) = SnI_4(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	31.540	67.570	67.570	0	-51.460	-51.406	37.681
300*	31.570	67.770	67.570	.060	-51.460	-51.405	37.448
386.8	32.586	75.924	68.559	2.849	-51.664	-51.366	29.022
386.8	32.586	75.924	68.559	2.849	-59.082	-51.366	29.022
400	32.740	77.020	68.820	3.280	-59.251	-51.100	27.919
418	32.880	78.470	69.209	3.870	-59.480	-50.730	26.524
418	40.100	89.470	69.209	8.470	-54.880	-50.730	26.524
458.4	40.100	93.170	71.158	10.090	-55.101	-50.313	23.987
458.4	40.100	93.170	71.158	10.090	-75.143	-50.313	23.987
500	40.100	96.660	73.140	11.760	-74.518	-48.086	21.018
505.12	40.100	97.069	73.380	11.965	-74.442	-47.817	20.689
505.12	40.100	97.069	73.380	11.965	-76.122	-47.817	20.689
600	40.100	103.970	77.687	15.770	-74.676	-42.625	15.526
628	40.100	105.800	78.906	16.890	-74.251	-41.144	14.318
628	25.670	125.650	78.906	29.355	-61.786	-41.144	14.318
700	25.710	128.430	83.851	31.205	-61.723	-38.774	12.105
800	25.740	131.870	89.645	33.780	-61.630	-35.501	9.698
900	25.760	134.900	94.506	36.355	-61.543	-32.239	7.829
1000	25.770	137.620	98.690	38.930	-61.458	-28.994	6.337

*Data 300 to 418 K extrapolated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
418 K, melting point of SnI_4; ΔH° = 4.600 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
505.12 K, melting point of Sn; ΔH° = 1.680 kcal/mol.
628 K, boiling point of SnI_4; ΔH° = 12.465 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-418 K: $Cp^\circ = 33.683 + 0.934\times10^{-3}T - 2.153\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 33.683\times10^{-3}T + 0.467\times10^{-6}T^2 + 2.153\times10^{2}T^{-1} - 10.806$

418-628 K: $Cp^\circ = 40.096$

$H^\circ - H^\circ_{298} = 40.096\times10^{-3}T - 8.290$

628-1000 K: $Cp^\circ = 26.733 - 0.778\times10^{-3}T - 2.268\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 26.733\times10^{-3}T - 0.389\times10^{-6}T^2 + 2.268\times10^{2}T^{-1} + 12.359$

SnI_4(c,l,g) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -52.658 + 2.961\times10^{-3}T - 4.859\times10^{-6}T^2 + 222.900T^{-1}$

$\Delta Gf^\circ = -52.658 - 2.961\times10^{-3}T\ln T + 4.859\times10^{-6}T^2 + 111.450T^{-1} + 18.370\times10^{-3}T$

386.8-418 K: $\Delta Hf^\circ = -55.569 - 9.847\times10^{-3}T - 1.875\times10^{-6}T^2 + 222.900T^{-1}$

$\Delta Gf^\circ = -55.569 + 9.847\times10^{-3}T\ln T + 1.875\times10^{-6}T^2 + 111.450T^{-1} - 49.261\times10^{-3}T$

418-458.4 K: $\Delta Hf^\circ = -53.053 - 3.434\times10^{-3}T - 2.342\times10^{-6}T^2 + 7.600T^{-1}$

$\Delta Gf^\circ = -53.053 + 3.434\times10^{-3}T\ln T + 2.342\times10^{-6}T^2 + 3.800T^{-1} - 16.153\times10^{-3}T$

458.4-505.12 K: $\Delta Hf^\circ = -82.479 + 17.246\times10^{-3}T - 2.478\times10^{-6}T^2 - 23.000T^{-1}$

$\Delta Gf^\circ = -82.479 - 17.246\times10^{-3}T\ln T + 2.478\times10^{-6}T^2 - 11.500T^{-1} + 174.772\times10^{-3}T$

505.12-628 K: $\Delta Hf^\circ = -84.445 + 16.023\times10^{-3}T - 0.317\times10^{-6}T^2 + 154.800T^{-1}$

$\Delta Gf^\circ = -84.445 - 16.023\times10^{-3}T\ln T + 0.317\times10^{-6}T^2 + 77.400T^{-1} + 171.794\times10^{-3}T$

628-1000 K: $\Delta Hf^\circ = -63.796 + 2.660\times10^{-3}T - 0.706\times10^{-6}T^2 + 381.600T^{-1}$

$\Delta Gf^\circ = -63.796 - 2.660\times10^{-3}T\ln T + 0.706\times10^{-6}T^2 + 190.800T^{-1} + 52.290\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Cartwright (21). Low-temperature heat capacities and entropy at 298 K from Anisimov (6). Data 300 to 418 K based on extrapolated heat capacities. Fusion data and heat capacity of liquid from Kelley (117). Data for gas from Ananthanarayanan (4).

$SnI_4(g)$

Tin Tetraiodide (ideal gas)

[Formation: $Sn(\beta,l) + 2I_2(c,l,g) = SnI_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	25.170	106.660	106.660	0	-30.520	-42.120	30.875
300	25.180	106.820	106.670	.045	-30.535	-42.195	30.738
386.8	25.423	113.246	107.444	2.244	-31.328	-45.467	25.689
386.8	25.423	113.246	107.444	2.244	-38.746	-45.467	25.689
400	25.460	114.100	107.650	2.580	-39.011	-45.692	24.965
458.4	25.536	117.579	108.697	4.072	-40.180	-46.581	22.208
458.4	25.536	117.579	108.697	4.072	-60.222	-46.581	22.208
500	25.590	119.800	109.530	5.135	-60.203	-45.341	19.818
505.12	25.594	120.061	109.635	5.266	-60.202	-45.190	19.552
505.12	25.594	120.061	109.635	5.266	-61.882	-45.190	19.552
600	25.660	124.470	111.645	7.695	-61.811	-42.060	15.320
700	25.710	128.430	113.766	10.265	-61.723	-38.774	12.105
800	25.740	131.870	115.820	12.840	-61.630	-35.501	9.698
900	25.760	134.900	117.772	15.415	-61.543	-32.239	7.829
1000	25.770	137.620	119.630	17.990	-61.458	-28.994	6.337

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
505.12 K, melting point of Sn; $\Delta H°$ = 1.680 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp° = 25.859 - 0.038\times10^{-3}T - 0.602\times10^{5}T^{-2}$

$H°- H°_{298} = 25.859\times10^{-3}T - 0.019\times10^{-6}T^2 + 0.602\times10^{2}T^{-1} - 7.910$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -28.822 - 4.863\times10^{-3}T - 5.345\times10^{-6}T^2 + 67.800T^{-1}$

$\Delta Gf° = -28.822 + 4.863\times10^{-3}T\ln T + 5.345\times10^{-6}T^2 + 33.900T^{-1} - 74.284\times10^{-3}T$

386.8-458.4 K: $\Delta Hf° = -31.733 - 17.671\times10^{-3}T - 2.361\times10^{-6}T^2 + 67.800T^{-1}$

$\Delta Gf° = -31.733 + 17.671\times10^{-3}T\ln T + 2.361\times10^{-6}T^2 + 33.900T^{-1} - 141.915\times10^{-3}T$

458.4-505.12 K: $\Delta Hf° = -61.159 + 3.009\times10^{-3}T - 2.497\times10^{-6}T^2 + 37.200T^{-1}$

$\Delta Gf° = -61.159 - 3.009\times10^{-3}T\ln T + 2.497\times10^{-6}T^2 + 18.600T^{-1} + 49.011\times10^{-3}T$

505.12-1000 K: $\Delta Hf° = -63.125 + 1.786\times10^{-3}T - 0.336\times10^{-6}T^2 + 215.000T^{-1}$

$\Delta Gf° = -63.125 - 1.786\times10^{-3}T\ln T + 0.336\times10^{-6}T^2 + 107.500T^{-1} + 46.033\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Zhamskaya (271). Other data from Ananthanarayanan (4).

SrBr(g)

Strontium Monobromide (ideal gas)

[Formation: $Sr(c,l,g) + 0.5Br_2(l,g) = SrBr(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.809	63.011	63.011	0	-21.300	-30.937	22.677
300	8.811	63.065	63.012	.016	-21.312	-30.996	22.581
332.6	8.838	63.975	63.062	.304	-21.530	-32.038	21.051
332.6	8.838	63.975	63.062	.304	-25.062	-32.038	21.051
400	8.895	65.613	63.358	.902	-25.206	-33.439	18.270
500	8.942	67.604	64.016	1.794	-25.454	-35.469	15.504
600	8.974	69.237	64.754	2.690	-25.744	-37.446	13.639
700	8.998	70.622	65.495	3.589	-26.083	-39.370	12.292
800	9.018	71.825	66.212	4.490	-26.478	-41.241	11.267
828	9.023	72.135	66.408	4.743	-26.600	-41.756	11.021
828	9.023	72.135	66.408	4.743	-26.780	-41.756	11.021
900	9.036	72.888	66.897	5.392	-27.102	-43.045	10.453
1000	9.053	73.841	67.544	6.297	-27.547	-44.792	9.789
1041	9.059	74.205	67.799	6.668	-27.729	-45.495	9.551
1041	9.059	74.205	67.799	6.668	-29.689	-45.495	9.551
1100	9.068	74.705	68.157	7.203	-29.916	-46.385	9.216
1200	9.083	75.494	68.736	8.110	-30.301	-47.865	8.717
1300	9.097	76.222	69.284	9.019	-30.684	-49.314	8.290
1400	9.111	76.897	69.804	9.930	-31.066	-50.732	7.919
1500	9.125	77.526	70.298	10.842	-31.448	-52.124	7.594
1600	9.140	78.115	70.768	11.755	-31.830	-53.488	7.306
1654.1	9.148	78.420	71.014	12.250	-32.036	-54.219	7.164
1654.1	9.148	78.420	71.014	12.250	-64.766	-54.219	7.164
1700	9.154	78.670	71.217	12.670	-64.784	-53.927	6.933
1800	9.170	79.193	71.645	13.586	-64.821	-53.286	6.470
1900	9.187	79.690	72.056	14.504	-64.859	-52.643	6.055
2000	9.205	80.161	72.450	15.423	-64.899	-52.000	5.682

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
828 K, α - γ transition point of Sr; $\Delta H°$ = 0.180 kcal/mol.
1041 K, melting point of Sr; $\Delta H°$ = 1.960 kcal/mol.
1654.1 K, boiling point of Sr; $\Delta H°$ = 32.730 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p° = 8.934 + 0.134\times10^{-3}T - 0.146\times10^{5}T^{-2}$

$H°- H°_{298} = 8.934\times10^{-3}T + 0.067\times10^{-6}T^{2} + 0.146\times10^{2}T^{-1} - 2.719$

SrBr(g) - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -19.818 - 4.705\times10^{-3}T - 2.415\times10^{-6}T^2 + 40.300T^{-1}$

$\Delta Gf^\circ = -19.818 + 4.705\times10^{-3}T\ln T + 2.415\times10^{-6}T^2 + 20.150T^{-1} - 65.050\times10^{-3}T$

332.6-828 K: $\Delta Hf^\circ = -24.818 - 0.125\times10^{-3}T - 2.493\times10^{-6}T^2 + 24.600T^{-1}$

$\Delta Gf^\circ = -24.818 + 0.125\times10^{-3}T\ln T + 2.493\times10^{-6}T^2 + 12.300T^{-1} - 23.373\times10^{-3}T$

828-1041 K: $\Delta Hf^\circ = -23.054 - 4.531\times10^{-3}T + 0.040\times10^{-6}T^2 - 1.100T^{-1}$

$\Delta Gf^\circ = -23.054 + 4.531\times10^{-3}T\ln T - 0.040\times10^{-6}T^2 - 0.550T^{-1} - 52.991\times10^{-3}T$

1041-1654.1 K: $\Delta Hf^\circ = -25.639 - 3.931\times10^{-3}T + 0.040\times10^{-6}T^2 - 1.100T^{-1}$

$\Delta Gf^\circ = -25.639 + 3.931\times10^{-3}T\ln T - 0.040\times10^{-6}T^2 - 0.550T^{-1} - 46.340\times10^{-3}T$

1654.1-2000 K: $\Delta Hf^\circ = -54.516 - 5.804\times10^{-3}T + 1.014\times10^{-6}T^2 - 5661.800T^{-1}$

$\Delta Gf^\circ = -54.516 + 5.804\times10^{-3}T\ln T - 1.014\times10^{-6}T^2 - 2830.900T^{-1} - 40.115\times10^{-3}T$

Source: Data from Chase (26).

$SrBr_2(c,l)$
Strontium Dibromide
[Formation: $Sr(c,l,g) + Br_2(l,g) = SrBr_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	18.368	34.282	34.282	0	-171.600	-167.248	122.594
300*	18.380	34.396	34.283	.034	-171.611	-167.221	121.818
332.6	18.546	36.301	34.389	.636	-171.808	-166.734	109.558
332.6	18.546	36.301	34.389	.636	-178.873	-166.734	109.558
400	18.890	39.755	35.010	1.898	-178.648	-164.298	89.767
500	19.320	44.017	36.399	3.809	-178.318	-160.748	70.262
600	19.760	47.577	37.974	5.762	-177.995	-157.265	57.283
700	20.290	50.661	39.571	7.763	-177.678	-153.836	48.029
800	20.930	53.410	41.131	9.823	-177.361	-150.451	41.101
828	21.160	54.134	41.559	10.412	-177.272	-149.511	39.463
828	21.160	54.134	41.559	10.412	-177.452	-149.511	39.463
900	21.750	55.921	42.638	11.955	-177.205	-147.092	35.718
918	21.920	56.354	42.901	12.350	-177.134	-146.489	34.874
918	27.500	59.535	42.901	15.270	-174.214	-146.489	34.874
930	27.500	59.892	43.118	15.600	-174.100	-146.127	34.339
930	27.818	62.496	43.118	18.022	-171.678	-146.127	34.339
1000	27.818	64.515	44.546	19.969	-170.991	-144.229	31.521
1041	27.818	65.633	45.355	21.110	-170.589	-143.140	30.051
1041	27.818	65.633	45.355	21.110	-172.549	-143.140	30.051
1100	27.818	67.166	46.483	22.751	-171.935	-141.489	28.111
1200	27.818	69.587	48.310	25.532	-170.897	-138.768	25.273
1300	27.818	71.814	50.034	28.314	-169.860	-136.134	22.886
1400	27.818	73.875	51.664	31.096	-168.824	-133.576	20.852
1500	27.818	75.794	53.209	33.878	-167.790	-131.096	19.100
1600	27.818	77.590	54.677	36.660	-166.757	-128.682	17.577
1654.1	27.818	78.515	55.442	38.164	-166.200	-127.406	16.833
1654.1	27.818	78.515	55.442	38.164	-198.930	-127.406	16.833
1700	27.818	79.276	56.075	39.441	-198.300	-125.431	16.125
1800	27.818	80.866	57.409	42.223	-196.927	-121.183	14.713
1900	27.818	82.370	58.683	45.005	-195.557	-117.009	13.459
2000	27.818	83.797	59.903	47.787	-194.191	-112.913	12.338

*Heat capacities 300-918 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
828 K, α - γ transition point of Sr; ΔH° = 0.180 kcal/mol.
918 K, α - β transition point of $SrBr_2$; ΔH° = 2.290 kcal/mol.
930 K, melting point of $SrBr_2$; ΔH° = 2.422 kcal/mol.
1041 K, melting point of Sr; ΔH° = 1.960 kcal/mol.
1654.1 K, boiling point of Sr; ΔH° = 32.730 kcal/mol.

$SrBr_2$(c,l) - Continued

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-918 K: $Cp^\circ = 16.522 + 5.482\times10^{-3}T + 0.188\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 16.522\times10^{-3}T + 2.741\times10^{-6}T^2 - 0.188\times10^{2}T^{-1} - 5.107$

918-930 K: $Cp^\circ = 27.500$

$H^\circ - H^\circ_{298} = 27.500\times10^{-3}T - 9.975$

930-2000 K: $Cp^\circ = 27.818$

$H^\circ - H^\circ_{298} = 27.818\times10^{-3}T - 7.849$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -169.813 - 6.163\times10^{-3}T + 0.309\times10^{-6}T^2 + 6.900T^{-1}$

$\Delta Gf^\circ = -169.813 + 6.163\times10^{-3}T\ln T - 0.309\times10^{-6}T^2 + 3.450T^{-1} - 26.457\times10^{-3}T$

332.6-828 K: $\Delta Hf^\circ = -179.814 + 2.998\times10^{-3}T + 0.154\times10^{-6}T^2 - 24.500T^{-1}$

$\Delta Gf^\circ = -179.814 - 2.998\times10^{-3}T\ln T - 0.154\times10^{-6}T^2 - 12.250T^{-1} + 56.898\times10^{-3}T$

828-918 K: $\Delta Hf^\circ = -178.050 - 1.408\times10^{-3}T + 2.686\times10^{-6}T^2 - 50.200T^{-1}$

$\Delta Gf^\circ = -178.050 + 1.408\times10^{-3}T\ln T - 2.686\times10^{-6}T^2 - 25.100T^{-1} + 27.279\times10^{-3}T$

918-930 K: $\Delta Hf^\circ = -182.919 + 9.570\times10^{-3}T - 0.055\times10^{-6}T^2 - 31.400T^{-1}$

$\Delta Gf^\circ = -182.919 - 9.570\times10^{-3}T\ln T + 0.055\times10^{-6}T^2 - 15.700T^{-1} + 104.949\times10^{-3}T$

930-1041 K: $\Delta Hf^\circ = -180.792 + 9.888\times10^{-3}T - 0.055\times10^{-6}T^2 - 31.400T^{-1}$

$\Delta Gf^\circ = -180.792 - 9.888\times10^{-3}T\ln T + 0.055\times10^{-6}T^2 - 15.700T^{-1} + 104.837\times10^{-3}T$

1041-1654.1 K: $\Delta Hf^\circ = -183.377 + 10.488\times10^{-3}T - 0.055\times10^{-6}T^2 - 31.400T^{-1}$

$\Delta Gf^\circ = -183.377 - 10.488\times10^{-3}T\ln T + 0.055\times10^{-6}T^2 - 15.700T^{-1} + 111.488\times10^{-3}T$

1654.1-2000 K: $\Delta Hf^\circ = -212.254 + 8.615\times10^{-3}T + 0.920\times10^{-6}T^2 - 5692.100T^{-1}$

$\Delta Gf^\circ = -212.254 - 8.615\times10^{-3}T\ln T - 0.920\times10^{-6}T^2 - 2846.050T^{-1} + 117.713\times10^{-3}T$

Source: Data from Chase (27) who estimated heat capacities 300-918 K and most molecular constants for gas.

$SrBr_2(g)$

Strontium Dibromide (ideal gas)

[Formation: $Sr(c,l,g) + Br_2(l,g) = SrBr_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	14.554	77.270	77.270	0	-97.300	-105.765	77.527
300	14.558	77.360	77.270	.027	-97.318	-105.817	77.086
332.6	14.606	78.864	77.354	.502	-97.641	-106.724	70.127
332.6	14.606	78.864	77.354	.502	-104.706	-106.724	70.127
400	14.704	81.571	77.843	1.491	-104.755	-107.131	58.533
500	14.774	84.861	78.931	2.965	-104.862	-107.715	47.081
600	14.813	87.558	80.150	4.445	-105.012	-108.271	39.437
700	14.837	89.844	81.377	5.927	-105.214	-108.800	33.968
800	14.852	91.826	82.561	7.412	-105.472	-109.294	29.857
828	14.855	92.337	82.883	7.828	-105.556	-109.427	28.883
828	14.855	92.337	82.883	7.828	-105.736	-109.427	28.883
900	14.863	93.576	83.689	8.898	-105.962	-109.738	26.648
1000	14.871	95.142	84.757	10.385	-106.275	-110.140	24.071
1041	14.873	95.740	85.178	10.995	-106.404	-110.295	23.155
1041	14.873	95.740	85.178	10.995	-108.364	-110.295	23.155
1100	14.877	96.560	85.767	11.872	-108.514	-110.402	21.934
1200	14.881	97.855	86.722	13.360	-108.769	-110.562	20.136
1300	14.884	99.046	87.624	14.848	-109.026	-110.702	18.610
1400	14.887	100.149	88.480	16.337	-109.283	-110.819	17.299
1500	14.889	101.176	89.293	17.825	-109.543	-110.922	16.161
1600	14.891	102.137	90.066	19.314	-109.803	-111.003	15.162
1654.1	14.892	102.632	90.468	20.120	-109.944	-111.043	14.671
1654.1	14.892	102.632	90.468	20.120	-142.674	-111.043	14.671
1700	14.892	103.040	90.802	20.804	-142.637	-110.167	14.163
1800	14.894	103.891	91.506	22.293	-142.557	-108.258	13.144
1900	14.895	104.697	92.180	23.782	-142.480	-106.353	12.233
2000	14.895	105.461	92.825	25.272	-142.406	-104.456	11.414

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
828 K, α - γ transition point of Sr; ΔH° = 0.180 kcal/mol.
1041 K, melting point of Sr; ΔH° = 1.960 kcal/mol.
1654.1 K, boiling point of Sr; ΔH° = 32.730 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 14.894 + 0.006\times10^{-3}T - 0.304\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.894\times10^{-3}T + 0.003\times10^{-6}T^2 + 0.304\times10^{2}T^{-1} - 4.543$

$SrBr_2(g)$ - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -94.949 - 7.791\times10^{-3}T - 2.429\times10^{-6}T^2 + 56.100T^{-1}$

$\Delta Gf^\circ = -94.949 + 7.791\times10^{-3}T\ln T + 2.429\times10^{-6}T^2 + 28.050T^{-1} - 81.705\times10^{-3}T$

332.6-828 K: $\Delta Hf^\circ = -104.950 + 1.370\times10^{-3}T - 2.584\times10^{-6}T^2 + 24.700T^{-1}$

$\Delta Gf^\circ = -104.950 - 1.370\times10^{-3}T\ln T + 2.584\times10^{-6}T^2 + 12.350T^{-1} + 1.650\times10^{-3}T$

828-1041 K: $\Delta Hf^\circ = -103.186 - 3.036\times10^{-3}T - 0.052\times10^{-6}T^2 - 1.000T^{-1}$

$\Delta Gf^\circ = -103.186 + 3.036\times10^{-3}T\ln T + 0.052\times10^{-6}T^2 - 0.500T^{-1} - 27.968\times10^{-3}T$

1041-1654.1 K: $\Delta Hf^\circ = -105.771 - 2.436\times10^{-3}T - 0.052\times10^{-6}T^2 - 1.000T^{-1}$

$\Delta Gf^\circ = -105.771 + 2.436\times10^{-3}T\ln T + 0.052\times10^{-6}T^2 - 0.500T^{-1} - 21.316\times10^{-3}T$

1654.1-2000 K: $\Delta Hf^\circ = -134.648 - 4.309\times10^{-3}T + 0.923\times10^{-6}T^2 - 5661.700T^{-1}$

$\Delta Gf^\circ = -134.648 + 4.309\times10^{-3}T\ln T - 0.923\times10^{-6}T^2 - 2830.850T^{-1} - 15.092\times10^{-3}T$

Source: Data from Chase (27) who estimated most molecular constants.

SrCl(g)

Strontium Monochloride (ideal gas)

[Formation: $Sr(c,l,g) + 0.5Cl_2(g) = SrCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.664	60.270	60.270	0	-29.600	-35.898	26.314
300	8.668	60.324	60.271	.016	-29.604	-35.938	26.180
400	8.809	62.839	60.611	.891	-29.802	-38.019	20.773
500	8.884	64.814	61.262	1.776	-30.043	-40.047	17.504
600	8.932	66.438	61.993	2.667	-30.329	-42.022	15.306
700	8.967	67.818	62.729	3.562	-30.663	-43.945	13.720
800	8.993	69.017	63.442	4.460	-31.057	-45.817	12.517
828	8.999	69.326	63.636	4.712	-31.178	-46.332	12.229
828	8.999	69.326	63.636	4.712	-31.358	-46.332	12.229
900	9.015	70.077	64.121	5.360	-31.679	-47.620	11.564
1000	9.035	71.028	64.765	6.263	-32.123	-49.367	10.789
1041	9.042	71.391	65.019	6.634	-32.305	-50.069	10.512
1041	9.042	71.391	65.019	6.634	-34.265	-50.069	10.512
1100	9.053	71.890	65.375	7.167	-34.491	-50.960	10.125
1200	9.069	72.679	65.951	8.073	-34.875	-52.441	9.551
1300	9.085	73.405	66.497	8.981	-35.258	-53.888	9.059
1400	9.100	74.079	67.015	9.890	-35.641	-55.307	8.634
1500	9.114	74.707	67.506	10.801	-36.023	-56.698	8.261
1600	9.129	75.296	67.975	11.713	-36.405	-58.063	7.931
1654.1	9.137	75.600	68.220	12.207	-36.611	-58.793	7.768
1654.1	9.137	75.600	68.220	12.207	-69.341	-58.793	7.768
1700	9.144	75.850	68.422	12.627	-69.360	-58.501	7.521
1800	9.160	76.373	68.850	13.542	-69.398	-57.861	7.025
1900	9.176	76.869	69.259	14.459	-69.437	-57.217	6.581
2000	9.194	77.340	69.651	15.377	-69.479	-56.574	6.182

Phase changes: 828 K, α - γ transition point of Sr; ΔH° = 0.180 kcal/mol.
1041 K, melting point of Sr; ΔH° = 1.960 kcal/mol.
1654.1 K, boiling point of Sr; ΔH° = 32.730 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.924 + 0.136\times10^{-3}T - 0.267\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.924\times10^{-3}T + 0.068\times10^{-6}T^2 + 0.267\times10^{2}T^{-1} - 2.756$

Formation equations (kcal/mol):

298.15-828 K: $\Delta Hf^\circ = -29.413 - 0.084\times10^{-3}T - 2.508\times10^{-6}T^2 + 18.250T^{-1}$

$\Delta Gf^\circ = -29.413 + 0.084\times10^{-3}T\ln T + 2.508\times10^{-6}T^2 + 9.125T^{-1} - 23.077\times10^{-3}T$

828-1041 K: $\Delta Hf^\circ = -27.650 - 4.490\times10^{-3}T + 0.024\times10^{-6}T^2 - 7.450T^{-1}$

$\Delta Gf^\circ = -27.650 + 4.490\times10^{-3}T\ln T - 0.024\times10^{-6}T^2 - 3.725T^{-1} - 52.695\times10^{-3}T$

1041-1654.1 K: $\Delta Hf^\circ = -30.235 - 3.890\times10^{-3}T + 0.024\times10^{-6}T^2 - 7.450T^{-1}$

$\Delta Gf^\circ = -30.235 + 3.890\times10^{-3}T\ln T - 0.024\times10^{-6}T^2 - 3.725T^{-1} - 46.044\times10^{-3}T$

1654.1-2000 K: $\Delta Hf^\circ = -59.112 - 5.763\times10^{-3}T + 0.999\times10^{-6}T^2 - 5668.150T^{-1}$

$\Delta Gf^\circ = -59.112 + 5.763\times10^{-3}T\ln T - 0.999\times10^{-6}T^2 - 2834.075T^{-1} - 39.820\times10^{-3}T$

Source: Data from Chase (27).

$SrCl_2$(c,l)
Strontium Dichloride
[Formation: $Sr(c,l,g) + Cl_2(g) = SrCl_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.070	27.450	27.450	0	-198.100	-186.669	136.830
300	18.087	27.562	27.452	.033	-198.094	-186.599	135.935
400	18.952	32.891	28.171	1.888	-197.728	-182.821	99.887
500	19.353	37.170	29.558	3.806	-197.362	-179.136	78.299
600	19.853	40.735	31.130	5.763	-197.016	-175.523	63.934
700	20.741	43.861	32.731	7.791	-196.657	-171.971	53.691
800	21.570	46.684	34.301	9.906	-196.276	-168.471	46.024
828	22.471	47.442	34.733	10.523	-196.157	-167.500	44.211
828	22.471	47.442	34.733	10.523	-196.337	-167.500	44.211
900	24.788	49.350	35.824	12.173	-195.976	-165.004	40.068
990	40.604	52.279	37.178	14.950	-194.813	-161.952	35.752
990	57.671	52.279	37.178	14.950	-194.813	-161.952	35.752
1000	51.111	52.825	37.332	15.493	-194.450	-161.622	35.322
1041	41.608	54.688	37.979	17.394	-193.286	-160.299	33.653
1041	41.608	54.688	37.979	17.394	-195.246	-160.299	33.653
1100	27.932	56.151	38.910	18.965	-194.699	-158.329	31.457
1146	27.708	57.291	39.625	20.245	-194.219	-156.818	29.906
1146	23.900	60.729	39.625	24.185	-190.279	-156.818	29.906
1200	23.900	61.830	40.600	25.476	-189.928	-155.249	28.274
1300	23.900	63.743	42.308	27.866	-189.280	-152.386	25.618
1400	23.900	65.514	43.903	30.256	-188.634	-149.571	23.349
1500	23.900	67.163	45.399	32.646	-187.990	-146.805	21.389
1600	23.900	68.705	46.808	35.036	-187.348	-144.078	19.680
1654.1	23.900	69.500	47.537	36.329	-187.001	-142.620	18.844
1654.1	23.900	69.500	47.537	36.329	-219.731	-142.620	18.844
1700	23.900	70.154	48.139	37.426	-219.281	-140.488	18.061
1800	23.900	71.520	49.400	39.816	-218.300	-135.882	16.498
1900	23.900	72.812	50.598	42.206	-217.322	-131.326	15.106
2000	23.900	74.038	51.740	44.596	-216.349	-126.827	13.859

Phase changes: 828 K, α - γ transition point of Sr; $\Delta H°$ = 0.180 kcal/mol.
990 K, second order transition point of $SrCl_2$; $\Delta H°$ = 0 kcal/mol.
1041 K, melting point of Sr; $\Delta H°$ = 1.960 kcal/mol.
1146 K, melting point of $SrCl_2$; $\Delta H°$ = 3.940 kcal/mol.
1654.1 K, boiling point of Sr; $\Delta H°$ = 32.730 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-990 K: $Cp° = 7.993 + 19.090\times10^{-3}T + 3.899\times10^{5}T^{-2}$

$H°- H°_{298} = 7.993\times10^{-3}T + 9.545\times10^{-6}T^2 - 3.899\times10^{2}T^{-1} - 1.924$

990-1146 K: $Cp° = 152.708 - 111.204\times10^{-3}T$

$H°- H°_{298} = 152.708\times10^{-3}T - 55.602\times10^{-6}T^2 - 81.735$

1146-2000 K: $Cp° = 23.900$

$H°- H°_{298} = 23.900\times10^{-3}T - 3.204$

$SrCl_2$(c,l) - Continued

Formation equations (kcal/mol):

298.15-828 K: $\Delta Hf^\circ = -195.647 - 5.428\times10^{-3}T + 6.925\times10^{-6}T^2 - 432.500T^{-1}$

$\Delta Gf^\circ = -195.647 + 5.428\times10^{-3}T\ln T - 6.925\times10^{-6}T^2 - 216.250T^{-1} + 3.682\times10^{-3}T$

828-990 K: $\Delta Hf^\circ = -193.883 - 9.834\times10^{-3}T + 9.457\times10^{-6}T^2 - 458.200T^{-1}$

$\Delta Gf^\circ = -193.883 + 9.834\times10^{-3}T\ln T - 9.457\times10^{-6}T^2 - 229.100T^{-1} - 25.936\times10^{-3}T$

990-1041 K: $\Delta Hf^\circ = -273.694 + 134.881\times10^{-3}T - 55.690\times10^{-6}T^2 - 68.300T^{-1}$

$\Delta Gf^\circ = -273.694 - 134.881\times10^{-3}T\ln T + 55.690\times10^{-6}T^2 - 34.150T^{-1} + 988.188\times10^{-3}T$

1041-1146 K: $\Delta Hf^\circ = -276.279 + 135.481\times10^{-3}T - 55.690\times10^{-6}T^2 - 68.300T^{-1}$

$\Delta Gf^\circ = -276.279 - 135.481\times10^{-3}T\ln T + 55.690\times10^{-6}T^2 - 34.150T^{-1} + 994.840\times10^{-3}T$

1146-1654.1 K: $\Delta Hf^\circ = -197.748 + 6.673\times10^{-3}T - 0.088\times10^{-6}T^2 - 68.300T^{-1}$

$\Delta Gf^\circ = -197.748 - 6.673\times10^{-3}T\ln T + 0.088\times10^{-6}T^2 - 34.150T^{-1} + 82.705\times10^{-3}T$

1654.1-2000 K: $\Delta Hf^\circ = -226.625 + 4.800\times10^{-3}T + 0.887\times10^{-6}T^2 - 5729.000T^{-1}$

$\Delta Gf^\circ = -226.625 - 4.800\times10^{-3}T\ln T - 0.887\times10^{-6}T^2 - 2864.500T^{-1} + 88.930\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (187). Low-temperature heat capacities and entropy at 298 K from Smith (216). High-temperature data based on Dworkin (67) and Efremova (93).

$SrCl_2(g)$

Strontium Dichloride (ideal gas)

[Formation: $Sr(c,l,g) + Cl_2(g) = SrCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	13.330	75.580	75.580	0	-113.100	-116.019	85.043
300	13.337	75.662	75.580	.025	-113.102	-116.037	84.532
400	13.575	79.536	76.106	1.372	-113.244	-116.995	63.922
500	13.692	82.579	77.107	2.736	-113.432	-117.911	51.538
600	13.757	85.082	78.235	4.108	-113.671	-118.787	43.267
700	13.797	87.205	79.368	5.486	-113.962	-119.617	37.346
800	13.823	89.050	80.466	6.867	-114.315	-120.403	32.892
828	13.828	89.526	80.765	7.254	-114.426	-120.614	31.836
828	13.828	89.526	80.765	7.254	-114.606	-120.614	31.836
900	13.841	90.679	81.511	8.251	-114.898	-121.122	29.412
1000	13.854	92.138	82.503	9.635	-115.308	-121.793	26.617
1041	13.858	92.695	82.894	10.203	-115.476	-122.055	25.624
1041	13.858	92.695	82.894	10.203	-117.436	-122.055	25.624
1100	13.864	93.459	83.440	11.021	-117.643	-122.311	24.301
1200	13.871	94.665	84.325	12.408	-117.996	-122.719	22.350
1300	13.877	95.776	85.164	13.795	-118.351	-123.100	20.695
1400	13.881	96.804	85.959	15.183	-118.707	-123.450	19.271
1500	13.885	97.762	86.714	16.572	-119.064	-123.777	18.034
1600	13.888	98.659	87.434	17.960	-119.424	-124.080	16.948
1654.1	13.890	99.121	87.809	18.711	-119.619	-124.234	16.414
1654.1	13.890	99.121	87.809	18.711	-152.349	-124.234	16.414
1700	13.891	99.501	88.119	19.349	-152.358	-123.455	15.871
1800	13.893	100.295	88.773	20.739	-152.377	-121.754	14.783
1900	13.895	101.046	89.400	22.128	-152.400	-120.049	13.809
2000	13.896	101.759	90.001	23.517	-152.428	-118.348	12.932

Phase changes: 828 K, α - γ transition point of Sr; ΔH° = 0.180 kcal/mol.
1041 K, melting point of Sr; ΔH° = 1.960 kcal/mol.
1654.1 K, boiling point of Sr; ΔH° = 32.730 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.886 + 0.014\times10^{-3}T - 0.498\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.886\times10^{-3}T + 0.007\times10^{-6}T^2 + 0.498\times10^{2}T^{-1} - 4.308$

Formation equations (kcal/mol):

298.15-828 K: $\Delta Hf^\circ = -113.031 + 0.465\times10^{-3}T - 2.613\times10^{-6}T^2 + 7.200T^{-1}$

$\Delta Gf^\circ = -113.031 - 0.465\times10^{-3}T\ln T + 2.613\times10^{-6}T^2 + 3.600T^{-1} - 8.193\times10^{-3}T$

828-1041 K: $\Delta Hf^\circ = -111.267 - 3.941\times10^{-3}T - 0.081\times10^{-6}T^2 - 18.500T^{-1}$

$\Delta Gf^\circ = -111.267 + 3.941\times10^{-3}T\ln T + 0.081\times10^{-6}T^2 - 9.250T^{-1} - 37.812\times10^{-3}T$

1041-1654.1 K: $\Delta Hf^\circ = -113.852 - 3.341\times10^{-3}T - 0.081\times10^{-6}T^2 - 18.500T^{-1}$

$\Delta Gf^\circ = -113.852 + 3.341\times10^{-3}T\ln T + 0.081\times10^{-6}T^2 - 9.250T^{-1} - 31.160\times10^{-3}T$

1654.1-2000 K: $\Delta Hf^\circ = -142.729 - 5.214\times10^{-3}T + 0.894\times10^{-6}T^2 - 5679.200T^{-1}$

$\Delta Gf^\circ = -142.729 + 5.214\times10^{-3}T\ln T - 0.894\times10^{-6}T^2 - 2839.600T^{-1} - 24.936\times10^{-3}T$

Source: Data from Chase (27).

SrF(g)

Strontium Monofluoride (ideal gas)

[Formation: $Sr(c,l,g) + 0.5F_2(g) = SrF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.242	57.315	57.315	0	-70.400	-76.540	56.105
300	8.249	57.366	57.316	.015	-70.404	-76.578	55.787
400	8.529	59.782	57.642	.856	-70.606	-78.606	42.948
500	8.687	61.703	58.269	1.717	-70.846	-80.579	35.220
600	8.785	63.297	58.979	2.591	-71.130	-82.500	30.050
700	8.851	64.656	59.695	3.473	-71.463	-84.370	26.341
800	8.898	65.841	60.390	4.361	-71.854	-86.188	23.545
828	8.908	66.147	60.579	4.610	-71.975	-86.688	22.881
828	8.908	66.147	60.579	4.610	-72.155	-86.688	22.881
900	8.934	66.891	61.055	5.252	-72.475	-87.937	21.354
1000	8.963	67.834	61.687	6.147	-72.920	-89.631	19.589
1041	8.973	68.194	61.936	6.515	-73.103	-90.312	18.960
1041	8.973	68.194	61.936	6.515	-75.063	-90.312	18.960
1100	8.988	68.690	62.285	7.045	-75.289	-91.171	18.114
1200	9.009	69.473	62.852	7.945	-75.674	-92.597	16.864
1300	9.028	70.194	63.389	8.846	-76.061	-93.992	15.801
1400	9.045	70.864	63.900	9.750	-76.447	-95.357	14.886
1500	9.061	71.489	64.386	10.655	-76.834	-96.696	14.088
1600	9.077	72.074	64.848	11.562	-77.220	-98.005	13.387
1654.1	9.085	72.376	65.089	12.054	-77.428	-98.705	13.041
1654.1	9.085	72.376	65.089	12.054	-110.158	-98.705	13.041
1700	9.092	72.625	65.289	12.471	-110.179	-98.388	12.648
1800	9.107	73.145	65.711	13.381	-110.223	-97.693	11.861
1900	9.122	73.638	66.116	14.292	-110.268	-96.995	11.157
2000	9.139	74.106	66.504	15.205	-110.316	-96.296	10.523

Phase changes: 828 K, α - γ transition point of Sr; ΔH° = 0.180 kcal/mol.
1041 K, melting point of Sr; ΔH° = 1.960 kcal/mol.
1654.1 K, boiling point of Sr; ΔH° = 32.730 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.840 + 0.168\times10^{-3}T - 0.577\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.840\times10^{-3}T + 0.084\times10^{-6}T^2 + 0.577\times10^{2}T^{-1} - 2.837$

Formation equations (kcal/mol):

298.15-828 K: $\Delta Hf^\circ = -70.283 - 0.008\times10^{-3}T - 2.535\times10^{-6}T^2 + 33.150T^{-1}$

$\Delta Gf^\circ = -70.283 + 0.008\times10^{-3}T\ln T + 2.535\times10^{-6}T^2 + 16.575T^{-1} - 21.972\times10^{-3}T$

828-1041 K: $\Delta Hf^\circ = -68.520 - 4.414\times10^{-3}T - 0.003\times10^{-6}T^2 + 7.450T^{-1}$

$\Delta Gf^\circ = -68.520 + 4.414\times10^{-3}T\ln T + 0.003\times10^{-6}T^2 + 3.725T^{-1} - 51.591\times10^{-3}T$

1041-1654.1 K: $\Delta Hf^\circ = -71.105 - 3.814\times10^{-3}T - 0.003\times10^{-6}T^2 + 7.450T^{-1}$

$\Delta Gf^\circ = -71.105 + 3.814\times10^{-3}T\ln T + 0.003\times10^{-6}T^2 + 3.725T^{-1} - 44.939\times10^{-3}T$

1654.1-2000 K: $\Delta Hf^\circ = -99.982 - 5.687\times10^{-3}T + 0.972\times10^{-6}T^2 - 5653.250T^{-1}$

$\Delta Gf^\circ = -99.982 + 5.687\times10^{-3}T\ln T - 0.972\times10^{-6}T^2 - 2826.625T^{-1} - 38.715\times10^{-3}T$

Source: Data from Chase (27).

$SrF_2(c,l)$
Strontium Difluoride
[Formation: $Sr(c,l,g) + F_2(g) = SrF_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	16.730	19.630	19.630	0	-290.700	-278.383	204.057
300	16.753	19.734	19.631	.031	-290.695	-278.307	202.744
400	17.791	24.699	20.299	1.760	-290.394	-274.220	149.825
500	18.625	28.762	21.598	3.582	-290.075	-270.214	118.109
600	19.239	32.216	23.088	5.477	-289.752	-266.273	96.989
700	19.588	35.211	24.610	7.421	-289.447	-262.384	81.919
800	19.712	37.837	26.103	9.387	-289.191	-258.537	70.628
828	19.728	38.515	26.512	9.939	-289.131	-257.466	67.957
828	19.728	38.515	26.512	9.939	-289.311	-257.466	67.957
900	19.769	40.161	27.538	11.361	-289.165	-254.700	61.849
1000	20.048	42.255	28.907	13.348	-288.958	-250.883	54.830
1041	20.428	43.068	29.449	14.178	-288.860	-249.324	52.343
1041	20.428	43.068	29.449	14.178	-290.820	-249.324	52.343
1100	20.975	44.202	30.209	15.392	-290.624	-246.976	49.069
1200	23.114	46.108	31.455	17.584	-290.163	-243.027	44.261
1300	27.171	48.103	32.658	20.079	-289.403	-239.127	40.200
1400	33.989	50.346	33.839	23.110	-288.112	-235.304	36.732
1480	42.089	52.445	34.786	26.135	-286.481	-232.330	34.307
1480	35.628	52.445	34.786	26.135	-286.481	-232.330	34.307
1500	34.851	52.918	35.025	26.840	-286.125	-231.600	33.744
1600	30.964	55.044	36.212	30.131	-284.580	-228.017	31.145
1654.1	28.861	56.038	36.844	31.749	-283.907	-226.115	29.875
1654.1	28.861	56.038	36.844	31.749	-316.637	-226.115	29.875
1700	27.077	56.804	37.373	33.033	-316.000	-223.614	28.747
1750	25.133	57.562	37.939	34.340	-315.398	-220.905	27.588
1750	23.500	61.602	37.939	41.410	-308.328	-220.905	27.588
1800	23.500	62.264	38.606	42.585	-307.858	-218.414	26.519
1900	23.500	63.535	39.885	44.935	-306.921	-213.470	24.554
2000	23.500	64.740	41.097	47.285	-305.990	-208.576	22.792

Phase changes: 828 K, α - γ transition point of Sr; ΔH° = 0.180 kcal/mol.
1041 K, melting point of Sr; ΔH° = 1.960 kcal/mol.
1480 K, second order transition point of SrF_2; ΔH° = 0 kcal/mol.
1654.1 K, boiling point of Sr; ΔH° = 32.730 kcal/mol.
1750 K, melting point of SrF_2; ΔH° = 7.070 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1480 K: $Cp^\circ = 8.440 + 14.486\times10^{-3}T + 3.506\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.440\times10^{-3}T + 7.243\times10^{-6}T^2 - 3.506\times10^{2}T^{-1} - 1.984$

1480-1750 K: $Cp^\circ = 93.155 - 38.866\times10^{-3}T$

$H^\circ - H^\circ_{298} = 93.155\times10^{-3}T - 19.433\times10^{-6}T^2 - 69.168$

1750-2000 K: $Cp^\circ = 23.500$

$H^\circ - H^\circ_{298} = 23.500\times10^{-3}T + 0.285$

SrF_2(c,1) - Continued

Formation equations (kcal/mol):

298.15-828 K: $\Delta Hf^\circ = -288.287 - 4.662\times10^{-3}T + 4.537\times10^{-6}T^2 - 425.400T^{-1}$

$\Delta Gf^\circ = -288.287 + 4.662\times10^{-3}T\ln T - 4.537\times10^{-6}T^2 - 212.700T^{-1} + 10.402\times10^{-3}T$

828-1041 K: $\Delta Hf^\circ = -286.523 - 9.068\times10^{-3}T + 7.069\times10^{-6}T^2 - 451.100T^{-1}$

$\Delta Gf^\circ = -286.523 + 9.068\times10^{-3}T\ln T - 7.069\times10^{-6}T^2 - 225.550T^{-1} - 19.217\times10^{-3}T$

1041-1480 K: $\Delta Hf^\circ = -289.108 - 8.468\times10^{-3}T + 7.069\times10^{-6}T^2 - 451.100T^{-1}$

$\Delta Gf^\circ = -289.108 + 8.468\times10^{-3}T\ln T - 7.069\times10^{-6}T^2 - 225.550T^{-1} - 12.565\times10^{-3}T$

1480-1654.1 K: $\Delta Hf^\circ = -356.292 + 76.247\times10^{-3}T - 19.607\times10^{-6}T^2 - 100.500T^{-1}$

$\Delta Gf^\circ = -356.292 - 76.247\times10^{-3}T\ln T + 19.607\times10^{-6}T^2 - 50.250T^{-1} + 611.671\times10^{-3}T$

1654.1-1750 K: $\Delta Hf^\circ = -385.169 + 74.374\times10^{-3}T - 18.632\times10^{-6}T^2 - 5761.200T^{-1}$

$\Delta Gf^\circ = -385.169 - 74.374\times10^{-3}T\ln T + 18.632\times10^{-6}T^2 - 2880.600T^{-1} + 617.896\times10^{-3}T$

1750-2000 K: $\Delta Hf^\circ = -315.716 + 4.719\times10^{-3}T + 0.801\times10^{-6}T^2 - 5761.200T^{-1}$

$\Delta Gf^\circ = -315.716 - 4.719\times10^{-3}T\ln T - 0.801\times10^{-6}T^2 - 2880.600T^{-1} + 92.076\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Parker (187). Low-temperature heat capacities and entropy at 298 K from Smith (216). High-temperature data based on Efremova (73).

$SrF_2(g)$

Strontium Difluoride (ideal gas)

[Formation: $Sr(c,l,g) + F_2(g) = SrF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	12.665	69.694	69.694	0	-183.100	-185.709	136.127
300	12.677	69.773	69.696	.023	-183.103	-185.726	135.300
400	13.153	73.493	70.198	1.318	-183.236	-186.580	101.941
500	13.405	76.457	71.163	2.647	-183.410	-187.396	81.910
600	13.551	78.915	72.257	3.995	-183.634	-188.174	68.542
700	13.642	81.012	73.362	5.355	-183.913	-188.910	58.980
800	13.703	82.838	74.434	6.723	-184.255	-189.602	51.796
828	13.715	83.310	74.726	7.107	-184.363	-189.788	50.094
828	13.715	83.310	74.726	7.107	-184.543	-189.788	50.094
900	13.746	84.454	75.460	8.095	-184.831	-190.230	46.194
1000	13.776	85.904	76.433	9.471	-185.235	-190.809	41.701
1041	13.785	86.458	76.817	10.036	-185.401	-191.034	40.106
1041	13.785	86.458	76.817	10.036	-187.361	-191.034	40.106
1100	13.799	87.218	77.354	10.850	-187.566	-191.236	37.995
1200	13.817	88.420	78.228	12.231	-187.916	-191.554	34.886
1300	13.830	89.526	79.054	13.613	-188.269	-191.843	32.251
1400	13.841	90.552	79.840	14.997	-188.625	-192.105	29.989
1500	13.850	91.507	80.586	16.382	-188.983	-192.342	28.024
1600	13.857	92.401	81.297	17.767	-189.344	-192.552	26.301
1654.1	13.860	92.862	81.667	18.517	-189.540	-192.657	25.455
1654.1	13.860	92.862	81.667	18.517	-222.270	-192.657	25.455
1700	13.863	93.241	81.975	19.153	-222.280	-191.836	24.662
1800	13.868	94.034	82.623	20.540	-222.303	-190.045	23.074
1900	13.873	94.784	83.243	21.927	-222.329	-188.251	21.653
2000	13.876	95.495	83.838	23.314	-222.361	-186.457	20.375

Phase changes: 828 K, α - γ transition point of Sr; $\Delta H° = 0.180$ kcal/mol.
1041 K, melting point of Sr; $\Delta H° = 1.960$ kcal/mol.
1654.1 K, boiling point of Sr; $\Delta H° = 32.730$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.776 + 0.084\times10^{-3}T - 1.010\times10^{5}T^{-2}$

$H°-H°_{298} = 13.776\times10^{-3}T + 0.042\times10^{-6}T^2 + 1.010\times10^{2}T^{-1} - 4.450$

Formation equations (kcal/mol):

298.15-828 K: $\Delta Hf° = -183.152 + 0.674\times10^{-3}T - 2.664\times10^{-6}T^2 + 26.200T^{-1}$

$\Delta Gf° = -183.152 - 0.674\times10^{-3}T\ln T + 2.664\times10^{-6}T^2 + 13.100T^{-1} - 5.678\times10^{-3}T$

828-1041 K: $\Delta Hf° = -181.389 - 3.732\times10^{-3}T - 0.132\times10^{-6}T^2 + 0.500T^{-1}$

$\Delta Gf° = -181.389 + 3.732\times10^{-3}T\ln T + 0.132\times10^{-6}T^2 + 0.250T^{-1} - 35.296\times10^{-3}T$

1041-1654.1 K: $\Delta Hf° = -183.973 - 3.132\times10^{-3}T - 0.132\times10^{-6}T^2 + 0.500T^{-1}$

$\Delta Gf° = -183.973 + 3.132\times10^{-3}T\ln T + 0.132\times10^{-6}T^2 + 0.250T^{-1} - 28.645\times10^{-3}T$

1654.1-2000 K: $\Delta Hf° = -212.851 - 5.005\times10^{-3}T + 0.843\times10^{-6}T^2 - 5660.200T^{-1}$

$\Delta Gf° = -212.851 + 5.005\times10^{-3}T\ln T - 0.843\times10^{-6}T^2 - 2830.100T^{-1} - 22.420\times10^{-3}T$

Source: Data from Chase (27).

SrI(g)

Strontium Monoiodide (ideal gas)

[Formation: $Sr(c,l,g) + 0.5I_2(c,l,g) = SrI(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	8.875	65.033	65.033	0	7.288	-4.237	3.106
300	8.877	65.088	65.035	.016	7.280	-4.309	3.139
386.8	8.932	67.352	65.310	.790	6.880	-7.610	4.300
386.8	8.932	67.352	65.310	.790	5.026	-7.610	4.300
400	8.940	67.652	65.382	.908	4.927	-8.040	4.393
458.4	8.962	68.872	65.750	1.431	4.484	-9.901	4.720
458.4	8.962	68.872	65.750	1.431	-.526	-9.901	4.720
500	8.978	69.651	66.043	1.804	-.635	-10.746	4.697
600	9.005	71.290	66.785	2.703	-.927	-12.743	4.641
700	9.028	72.680	67.531	3.604	-1.266	-14.687	4.585
800	9.048	73.887	68.252	4.508	-1.660	-16.578	4.529
828	9.053	74.198	68.448	4.761	-1.782	-17.098	4.513
828	9.053	74.198	68.448	4.761	-1.962	-17.098	4.513
900	9.067	74.954	68.938	5.414	-2.283	-18.400	4.468
1000	9.085	75.910	69.588	6.322	-2.728	-20.166	4.407
1041	9.092	76.275	69.844	6.695	-2.910	-20.876	4.383
1041	9.092	76.275	69.844	6.695	-4.870	-20.876	4.383
1100	9.102	76.777	70.203	7.231	-5.097	-21.779	4.327
1200	9.118	77.569	70.784	8.142	-5.480	-23.277	4.239
1300	9.135	78.300	71.335	9.055	-5.861	-24.745	4.160
1400	9.151	78.977	71.856	9.969	-6.243	-26.182	4.087
1500	9.168	79.609	72.352	10.885	-6.624	-27.595	4.021
1600	9.184	80.202	72.826	11.802	-7.004	-28.980	3.958
1654.1	9.194	80.507	73.071	12.300	-7.209	-29.720	3.927
1654.1	9.194	80.507	73.071	12.300	-39.939	-29.720	3.927
1700	9.202	80.759	73.275	12.722	-39.956	-29.437	3.784
1800	9.221	81.285	73.706	13.643	-39.992	-28.816	3.499
1900	9.241	81.784	74.118	14.566	-40.028	-28.193	3.243
2000	9.263	82.259	74.514	15.491	-40.065	-27.571	3.013

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
828 K, α - γ transition point of Sr; ΔH° = 0.180 kcal/mol.
1041 K, melting point of Sr; ΔH° = 1.960 kcal/mol.
1654.1 K, boiling point of Sr; ΔH° = 32.730 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.938 + 0.158\times10^{-3}T - 0.097\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.938\times10^{-3}T + 0.079\times10^{-6}T^2 + 0.097\times10^{2}T^{-1} - 2.704$

SrI(g) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = 8.078 - 2.095\times10^{-3}T - 3.199\times10^{-6}T^2 + 35.400T^{-1}$

$\Delta Gf^\circ = 8.078 + 2.095\times10^{-3}T\ln T + 3.199\times10^{-6}T^2 + 17.700T^{-1} - 54.391\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = 7.351 - 5.297\times10^{-3}T - 2.453\times10^{-6}T^2 + 35.400T^{-1}$

$\Delta Gf^\circ = 7.351 + 5.297\times10^{-3}T\ln T + 2.453\times10^{-6}T^2 + 17.700T^{-1} - 71.298\times10^{-3}T$

458.4-828 K: $\Delta Hf^\circ = -0.006 - 0.127\times10^{-3}T - 2.487\times10^{-6}T^2 + 27.750T^{-1}$

$\Delta Gf^\circ = -0.006 + 0.127\times10^{-3}T\ln T + 2.487\times10^{-6}T^2 + 13.875T^{-1} - 23.567\times10^{-3}T$

828-1041 K: $\Delta Hf^\circ = 1.757 - 4.533\times10^{-3}T + 0.045\times10^{-6}T^2 + 2.050T^{-1}$

$\Delta Gf^\circ = 1.757 + 4.533\times10^{-3}T\ln T - 0.045\times10^{-6}T^2 + 1.025T^{-1} - 53.185\times10^{-3}T$

1041-1654.1 K: $\Delta Hf^\circ = -0.827 - 3.933\times10^{-3}T + 0.045\times10^{-6}T^2 + 2.050T^{-1}$

$\Delta Gf^\circ = -0.827 + 3.933\times10^{-3}T\ln T - 0.045\times10^{-6}T^2 + 1.025T^{-1} - 46.534\times10^{-3}T$

1654.1-2000 K: $\Delta Hf^\circ = -29.705 - 5.806\times10^{-3}T + 1.020\times10^{-6}T^2 - 5658.650T^{-1}$

$\Delta Gf^\circ = -29.705 + 5.806\times10^{-3}T\ln T - 1.020\times10^{-6}T^2 - 2829.325T^{-1} - 40.309\times10^{-3}T$

Source: Data from Chase (27).

$SrI_2(c,l)$
Strontium Diiodide
[Formation: $Sr(c,l,g) + I_2(c,l,g) = SrI_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	18.630	38.031	38.031	0	-134.200	-133.536	97.883
300	18.650	38.146	38.033	.034	-134.202	-133.532	97.277
386.8	19.214	42.954	38.616	1.678	-134.336	-133.323	75.329
386.8	19.214	42.954	38.616	1.678	-138.045	-133.323	75.329
400	19.300	43.600	38.770	1.932	-138.135	-133.161	72.755
458.4	19.685	46.255	39.557	3.070	-138.525	-132.405	63.125
458.4	19.685	46.255	39.557	3.070	-148.546	-132.405	63.125
500	19.960	47.977	40.187	3.895	-148.389	-130.945	57.235
600	20.620	51.675	41.802	5.924	-147.999	-127.494	46.439
700	21.270	54.902	43.448	8.018	-147.595	-124.109	38.748
800	21.930	57.786	45.062	10.179	-147.183	-120.781	32.995
811	22.000	58.086	45.238	10.420	-147.139	-120.419	32.450
811	26.300	63.881	45.238	15.120	-142.439	-120.419	32.450
828	26.300	64.427	45.626	15.567	-142.297	-119.958	31.662
828	26.300	64.427	45.626	15.567	-142.477	-119.958	31.662
900	26.300	66.620	47.219	17.461	-141.882	-118.026	28.660
1000	26.300	69.391	49.300	20.091	-141.057	-115.418	25.224
1041	26.300	70.448	50.112	21.169	-140.719	-114.373	24.011
1041	26.300	70.448	50.112	21.169	-142.679	-114.373	24.011
1100	26.300	71.897	51.242	22.721	-142.158	-112.784	22.408
1200	26.300	74.186	53.060	25.351	-141.277	-110.153	20.061
1300	26.300	76.291	54.767	27.981	-140.396	-107.594	18.088
1400	26.300	78.240	56.375	30.611	-139.518	-105.103	16.407
1500	26.300	80.054	57.893	33.241	-138.641	-102.677	14.960
1600	26.300	81.752	59.333	35.871	-137.765	-100.306	13.701
1654.1	26.300	82.626	60.080	37.294	-137.293	-99.048	13.087
1654.1	26.300	82.626	60.080	37.294	-170.023	-99.048	13.087
1700	26.300	83.346	60.698	38.501	-169.465	-97.088	12.481
1800	26.300	84.849	61.998	41.131	-168.250	-92.864	11.275
1900	26.300	86.271	63.239	43.761	-167.039	-88.708	10.204
2000	26.300	87.620	64.425	46.391	-165.831	-84.617	9.246

*Heat capacities extrapolated 270-811 K.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
811 K, melting point of SrI_2; ΔH° = 4.700 kcal/mol.
828 K, α - γ transition point of Sr; ΔH° = 0.180 kcal/mol.
1041 K, melting point of Sr; ΔH° = 1.960 kcal/mol.
1654.1 K, boiling point of Sr; ΔH° = 32.730 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-811 K: $Cp^\circ = 16.692 + 6.548\times10^{-3}T - 0.013\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 16.692\times10^{-3}T + 3.274\times10^{-6}T^2 + 0.013\times10^{2}T^{-1} - 5.272$

811-2000 K: $Cp^\circ = 26.300$
$H^\circ - H^\circ_{298} = 26.300\times10^{-3}T - 6.209$

SrI_2(c,l) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -133.992 - 0.779\times10^{-3}T - 0.750\times10^{-6}T^2 + 27.000T^{-1}$

$\Delta Gf^\circ = -133.992 + 0.779\times10^{-3}T\ln T + 0.750\times10^{-6}T^2 + 13.500T^{-1} - 3.286\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -135.447 - 7.183\times10^{-3}T + 0.742\times10^{-6}T^2 + 27.000T^{-1}$

$\Delta Gf^\circ = -135.447 + 7.183\times10^{-3}T\ln T - 0.742\times10^{-6}T^2 + 13.500T^{-1} - 37.101\times10^{-3}T$

458.4-811 K: $\Delta Hf^\circ = -150.160 + 3.157\times10^{-3}T + 0.674\times10^{-6}T^2 + 11.700T^{-1}$

$\Delta Gf^\circ = -150.160 - 3.157\times10^{-3}T\ln T - 0.674\times10^{-6}T^2 + 5.850T^{-1} + 58.362\times10^{-3}T$

811-828 K: $\Delta Hf^\circ = -151.097 + 12.765\times10^{-3}T - 2.600\times10^{-6}T^2 + 10.400T^{-1}$

$\Delta Gf^\circ = -151.097 - 12.765\times10^{-3}T\ln T + 2.600\times10^{-6}T^2 + 5.200T^{-1} + 121.220\times10^{-3}T$

828-1041 K: $\Delta Hf^\circ = -149.334 + 8.359\times10^{-3}T - 0.068\times10^{-6}T^2 - 15.300T^{-1}$

$\Delta Gf^\circ = -149.334 - 8.359\times10^{-3}T\ln T + 0.068\times10^{-6}T^2 - 7.650T^{-1} + 91.602\times10^{-3}T$

1041-1654.1 K: $\Delta Hf^\circ = -151.918 + 8.959\times10^{-3}T - 0.068\times10^{-6}T^2 - 15.300T^{-1}$

$\Delta Gf^\circ = -151.918 - 8.959\times10^{-3}T\ln T + 0.068\times10^{-6}T^2 - 7.650T^{-1} + 98.253\times10^{-3}T$

1654.1-2000 K: $\Delta Hf^\circ = -180.796 + 7.086\times10^{-3}T + 0.907\times10^{-6}T^2 - 5676.000T^{-1}$

$\Delta Gf^\circ = -180.796 - 7.086\times10^{-3}T\ln T - 0.907\times10^{-6}T^2 - 2838.000T^{-1} + 104.478\times10^{-3}T$

Source: Data from Chase (27) who extrapolated heat capacities 270-811 K.

$SrI_2(g)$

Strontium Diiodide (ideal gas)

[Formation: $Sr(c,l,g) + I_2(c,l,g) = SrI_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	14.674	81.128	81.128	0	-65.700	-77.885	57.091
300	14.677	81.219	81.129	.027	-65.709	-77.961	56.794
386.8	14.761	84.960	81.586	1.305	-66.209	-81.444	46.017
386.8	14.761	84.960	81.586	1.305	-69.918	-81.444	46.017
400	14.774	85.456	81.706	1.500	-70.067	-81.835	44.712
458.4	14.801	87.471	82.315	2.364	-70.731	-83.505	39.812
458.4	14.801	87.471	82.315	2.364	-80.752	-83.505	39.812
500	14.820	88.758	82.798	2.980	-80.804	-83.751	36.607
600	14.845	91.463	84.023	4.464	-80.959	-84.327	30.716
700	14.861	93.753	85.254	5.949	-81.164	-84.873	26.498
800	14.871	95.738	86.443	7.436	-81.426	-85.385	23.326
828	14.873	96.250	86.766	7.852	-81.511	-85.522	22.573
828	14.873	96.250	86.766	7.852	-81.691	-85.522	22.573
900	14.878	97.489	87.575	8.923	-81.920	-85.846	20.846
1000	14.883	99.057	88.646	10.411	-82.237	-86.264	18.853
1041	14.884	99.655	89.068	11.021	-82.367	-86.426	18.144
1041	14.884	99.655	89.068	11.021	-84.327	-86.426	18.144
1100	14.886	100.476	89.659	11.899	-84.480	-86.543	17.194
1200	14.889	101.771	90.614	13.388	-84.740	-86.718	15.793
1300	14.891	102.963	91.519	14.877	-85.000	-86.872	14.604
1400	14.893	104.067	92.377	16.366	-85.263	-87.006	13.582
1500	14.894	105.094	93.190	17.856	-85.526	-87.122	12.694
1600	14.895	106.056	93.965	19.345	-85.791	-87.218	11.913
1654.1	14.896	106.551	94.369	20.151	-85.935	-87.266	11.530
1654.1	14.896	106.551	94.369	20.151	-118.665	-87.266	11.530
1700	14.896	106.959	94.703	20.835	-118.631	-86.396	11.107
1800	14.897	107.810	95.407	22.325	-118.556	-84.500	10.260
1900	14.898	108.616	96.082	23.814	-118.486	-82.610	9.502
2000	14.898	109.380	96.728	25.304	-118.418	-80.724	8.821

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
828 K, α - γ transition point of Sr; $\Delta H°$ = 0.180 kcal/mol.
1041 K, melting point of Sr; $\Delta H°$ = 1.960 kcal/mol.
1654.1 K, boiling point of Sr; $\Delta H°$ = 32.730 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:[2]

298.15-2000 K: $Cp° = 14.898 + 0.004\times10^{-3}T - 0.200\times10^{5}T^{-2}$

$H°- H°_{298} = 14.898\times10^{-3}T + 0.002\times10^{-6}T^{2} + 0.200\times10^{2}T^{-1} - 4.509$

$SrI_2(g)$ - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -64.729 - 2.573\times10^{-3}T - 4.022\times10^{-6}T^2 + 45.700T^{-1}$

$\Delta Gf^\circ = -64.729 + 2.573\times10^{-3}T\ln T + 4.022\times10^{-6}T^2 + 22.850T^{-1} - 60.244\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -66.184 - 8.977\times10^{-3}T - 2.530\times10^{-6}T^2 + 45.700T^{-1}$

$\Delta Gf^\circ = -66.184 + 8.977\times10^{-3}T\ln T + 2.530\times10^{-6}T^2 + 22.850T^{-1} - 94.059\times10^{-3}T$

458.4-828 K: $\Delta Hf^\circ = -80.897 + 1.363\times10^{-3}T - 2.598\times10^{-6}T^2 + 30.400T^{-1}$

$\Delta Gf^\circ = -80.897 - 1.363\times10^{-3}T\ln T + 2.598\times10^{-6}T^2 + 15.200T^{-1} + 1.403\times10^{-3}T$

828-1041 K: $\Delta Hf^\circ = -79.134 - 3.043\times10^{-3}T - 0.066\times10^{-6}T^2 + 4.700T^{-1}$

$\Delta Gf^\circ = -79.134 + 3.043\times10^{-3}T\ln T + 0.066\times10^{-6}T^2 + 2.350T^{-1} - 28.215\times10^{-3}T$

1041-1654.1 K: $\Delta Hf^\circ = -81.718 - 2.443\times10^{-3}T - 0.066\times10^{-6}T^2 + 4.700T^{-1}$

$\Delta Gf^\circ = -81.718 + 2.443\times10^{-3}T\ln T + 0.066\times10^{-6}T^2 + 2.350T^{-1} - 21.563\times10^{-3}T$

1654.1-2000 K: $\Delta Hf^\circ = -110.596 - 4.316\times10^{-3}T + 0.909\times10^{-6}T^2 - 5656.000T^{-1}$

$\Delta Gf^\circ = -110.596 + 4.316\times10^{-3}T\ln T - 0.909\times10^{-6}T^2 - 2828.000T^{-1} - 15.339\times10^{-3}T$

Source: Data from Chase (27) who estimated most molecular constants.

$TaBr_5(g)$

Tantalum Pentabromide (ideal gas)

[Formation: $Ta(c) + 2.5Br_2(l,g) = TaBr_5(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	30.320	109.030	109.030	0	-115.600	-118.034	86.520
300	30.340	109.220	109.037	.055	-115.638	-118.048	85.997
332.6	30.539	112.360	109.211	1.047	-116.315	-118.276	77.718
332.6	30.539	112.360	109.211	1.047	-133.977	-118.276	77.718
400	30.950	118.040	110.228	3.125	-133.790	-115.117	62.896
500	31.250	124.980	112.510	6.235	-133.510	-110.483	48.291
600	31.410	130.690	115.073	9.370	-133.225	-105.899	38.573
700	31.510	135.540	117.654	12.520	-132.943	-101.365	31.647
800	31.580	139.760	120.166	15.675	-132.667	-96.876	26.465
900	31.620	143.480	122.552	18.835	-132.403	-92.419	22.442
1000	31.650	146.810	124.820	21.990	-132.152	-87.996	19.231
1100	31.680	149.830	126.957	25.160	-131.897	-83.590	16.608
1200	31.700	152.590	128.986	28.325	-131.656	-79.215	14.427

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
538 K, melting point of $TaBr_5$; $\Delta H°$ = 10.9 kcal/mol.
618 K, boiling point of $TaBr_5$; $\Delta H°$ = 14.9 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $Cp° = 31.799 - 0.036\times10^{-3}T - 1.305\times10^{5}T^{-2}$

$H°- H°_{298} = 31.799\times10^{-3}T - 0.018\times10^{-6}T^2 + 1.305\times10^{2}T^{-1} - 9.917$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -110.665 - 18.485\times10^{-3}T - 0.450\times10^{-6}T^2 + 183.700T^{-1}$

$\Delta Gf° = -110.665 + 18.485\times10^{-3}T\ln T + 0.450\times10^{-6}T^2 + 91.850T^{-1} - 131.199\times10^{-3}T$

332.6-1200 K: $\Delta Hf° = -135.666 + 4.418\times10^{-3}T - 0.838\times10^{-6}T^2 + 105.200T^{-1}$

$\Delta Gf° = -135.666 - 4.418\times10^{-3}T\ln T + 0.838\times10^{-6}T^2 + 52.600T^{-1} + 77.188\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (254). Other data from So (218). Fusion and boiling data from Wiseman (266).

TaCl(g)

Tantalum Monochloride (ideal gas)

[Formation: $Ta(c) + 0.5Cl_2(g) = TaCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.360	61.940	61.940	0	86.000	78.434	-57.493
300	8.360	61.990	61.940	.016	85.997	78.389	-57.106
400	8.600	64.430	62.255	.870	85.821	75.885	-41.461
500	8.730	66.370	62.910	1.730	85.629	73.413	-32.088
600	8.810	67.970	63.620	2.610	85.445	70.990	-25.858
700	8.860	69.330	64.344	3.490	85.249	68.593	-21.415
800	8.900	70.510	65.035	4.380	85.054	66.233	-18.094
900	8.920	71.560	65.704	5.270	84.851	63.891	-15.515
1000	8.950	72.500	66.330	6.170	84.650	61.580	-13.458
1100	8.970	73.360	66.942	7.060	84.432	59.271	-11.776
1200	8.980	74.140	67.507	7.960	84.216	56.998	-10.381
1300	9.000	74.860	68.045	8.860	83.992	54.739	-9.202
1400	9.010	75.530	68.559	9.760	83.759	52.493	-8.194
1500	9.020	76.150	69.043	10.660	83.516	50.269	-7.324

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 8.838 + 0.154\times10^{-3}T - 0.466\times10^{5}T^{-2}$

$H°- H°_{298} = 8.838\times10^{-3}T + 0.077\times10^{-6}T^{2} + 0.466\times10^{2}T^{-1} - 2.798$

Formation equations (kcal/mol):

298.15-1500 K: $\Delta Hf° = 86.026 - 0.632\times10^{-3}T - 0.649\times10^{-6}T^{2} + 65.650T^{-1}$

$\Delta Gf° = 86.026 + 0.632\times10^{-3}T\ln T + 0.649\times10^{-6}T^{2} + 32.825T^{-1} - 29.622\times10^{-3}T$

Source: Data from Behrens (10).

$TaCl_2(g)$

Tantalum Dichloride (ideal gas)

[Formation: $Ta(c) + Cl_2(g) = TaCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	13.720	71.290	71.290	0	-16.000	-18.409	13.494
300	13.730	71.380	71.297	.025	-16.001	-18.425	13.422
400	14.190	75.390	71.815	1.430	-16.042	-19.217	10.499
500	14.430	78.590	72.870	2.860	-16.090	-20.009	8.746
600	14.570	81.230	74.047	4.310	-16.139	-20.786	7.571
700	14.650	83.490	75.247	5.770	-16.193	-21.563	6.732
800	14.710	85.450	76.400	7.240	-16.251	-22.325	6.099
900	14.750	87.180	77.502	8.710	-16.319	-23.079	5.604
1000	14.780	88.740	78.550	10.190	-16.387	-23.828	5.208
1100	14.800	90.150	79.541	11.670	-16.464	-24.568	4.881
1200	14.820	91.440	80.482	13.150	-16.550	-25.303	4.608
1300	14.830	92.620	81.366	14.630	-16.645	-26.022	4.375
1400	14.840	93.720	82.213	16.110	-16.750	-26.745	4.175
1500	14.850	94.750	83.017	17.600	-16.856	-27.458	4.001

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 14.832 + 0.032\times10^{-3}T - 0.997\times10^{5}T^{-2}$

$H°-H°_{298} = 14.832\times10^{-3}T + 0.016\times10^{-6}T^{2} + 0.997\times10^{2}T^{-1} - 4.758$

Formation equations (kcal/mol):

298.15-1500 K: $\Delta Hf° = -16.500 + 0.949\times10^{-3}T - 0.754\times10^{-6}T^{2} + 84.600T^{-1}$

$\Delta Gf° = -16.500 - 0.949\times10^{-3}T\ln T + 0.754\times10^{-6}T^{2} + 42.300T^{-1} - 1.698\times10^{-3}T$

Source: Data from Behrens (10).

$TaCl_3(g)$

Tantalum Trichloride (ideal gas)

[Formation: $Ta(c) + 1.5Cl_2(g) = TaCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.050	82.670	82.670	0	-77.000	-74.858	54.872
300	18.060	82.780	82.670	.033	-77.001	-74.844	54.523
400	18.780	88.090	83.390	1.880	-77.015	-74.124	40.499
500	19.140	92.320	84.760	3.780	-77.019	-73.396	32.081
600	19.360	95.830	86.330	5.700	-77.033	-72.676	26.472
700	19.490	98.820	87.891	7.650	-77.035	-71.939	22.460
800	19.580	101.430	89.430	9.600	-77.057	-71.216	19.455
900	19.640	103.740	90.896	11.560	-77.080	-70.485	17.116
1000	19.680	105.810	92.280	13.530	-77.104	-69.746	15.243
1100	19.710	107.690	93.599	15.500	-77.140	-69.012	13.711
1200	19.740	109.410	94.852	17.470	-77.186	-68.277	12.435
1300	19.760	110.990	96.036	19.440	-77.242	-67.536	11.354
1400	19.770	112.450	97.150	21.420	-77.299	-66.778	10.424
1500	19.790	113.820	98.220	23.400	-77.368	-66.030	9.620

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 19.664 + 0.152\times10^{-3}T - 1.475\times10^{5}T^{-2}$

$H°- H°_{298} = 19.664\times10^{-3}T + 0.076\times10^{-6}T^{2} + 1.475\times10^{2}T^{-1} - 6.364$

Formation equations (kcal/mol):

298.15-1500 K: $\Delta Hf° = -77.672 + 1.367\times10^{-3}T - 0.738\times10^{-6}T^{2} + 98.250T^{-1}$

$\Delta Gf° = -77.672 - 1.367\times10^{-3}T\ln T + 0.738\times10^{-6}T^{2} + 49.125T^{-1} + 16.457\times10^{-3}T$

Source: Data from Behrens (10).

$TaCl_4(g)$

Tantalum Tetrachloride (ideal gas)

[Formation: $Ta(c) + 2Cl_2(g) = TaCl_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	23.650	90.150	90.150	0	-137.090	-129.234	94.730
300	23.670	90.300	90.153	.044	-137.087	-129.185	94.110
400	24.540	97.240	91.090	2.460	-136.947	-126.572	69.155
500	24.980	102.770	92.890	4.940	-136.798	-123.992	54.196
600	25.230	107.350	94.933	7.450	-136.656	-121.447	44.237
700	25.380	111.250	96.993	9.980	-136.518	-118.924	37.129
800	25.490	114.640	98.990	12.520	-136.392	-116.420	31.804
900	25.560	117.650	100.894	15.080	-136.260	-113.926	27.665
1000	25.610	120.350	102.720	17.630	-136.152	-111.465	24.360
1100	25.650	122.790	104.426	20.200	-136.036	-108.991	21.654
1200	25.680	125.020	106.053	22.760	-135.942	-106.540	19.403
1300	25.700	127.080	107.595	25.330	-135.849	-104.096	17.500
1400	25.720	128.980	109.051	27.900	-135.768	-101.651	15.868
1500	25.730	130.760	110.440	30.480	-135.690	-99.217	14.456

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 25.606 + 0.168\times10^{-3}T - 1.783\times10^{5}T^{-2}$

$H°- H°_{298} = 25.606\times10^{-3}T + 0.084\times10^{-6}T^{2} + 1.783\times10^{2}T^{-1} - 8.240$

Formation equations (kcal/mol):

298.15-1500 K: $\Delta Hf° = -138.203 + 2.896\times10^{-3}T - 0.774\times10^{-6}T^{2} + 94.900T^{-1}$

$\Delta Gf° = -138.203 - 2.896\times10^{-3}T\ln T + 0.774\times10^{-6}T^{2} + 47.450T^{-1} + 45.819\times10^{-3}T$

Source: Data from Behrens (10).

$TaCl_5$(c,l,g)

Tantalum Pentachloride

[Formation: $Ta(c) + 2.5Cl_2(g) = TaCl_5(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	35.350	53.000	53.000	0	-205.300	-178.423	130.786
300	35.350	53.219	53.002	.065	-205.283	-178.256	129.858
400	35.350	63.388	54.388	3.600	-204.439	-169.379	92.543
489.7	35.350	70.540	56.713	6.771	-203.740	-161.588	72.115
489.7	51.960	87.693	56.713	15.171	-195.340	-161.588	72.115
500	51.760	88.774	57.364	15.705	-195.092	-160.881	70.320
506.9	51.590	89.484	57.797	16.062	-194.927	-160.411	69.160
506.9	30.600	114.485	57.797	28.735	-182.254	-160.411	69.160
600	30.931	119.675	67.005	31.602	-181.997	-156.420	56.975
700	31.153	124.461	74.880	34.707	-181.723	-152.179	47.512
800	31.300	128.631	81.343	37.830	-181.458	-147.979	40.425
900	31.401	132.324	86.807	40.965	-181.196	-143.809	34.921
1000	31.475	135.636	91.527	44.109	-180.941	-139.671	30.525
1100	31.530	138.639	95.675	47.260	-180.692	-135.555	26.932
1200	31.572	141.384	99.372	50.415	-180.453	-131.462	23.942
1300	31.604	143.913	102.702	53.574	-180.222	-127.389	21.416
1400	31.630	146.256	105.731	56.735	-180.002	-123.334	19.253
1500	31.651	148.439	108.506	59.899	-179.793	-119.294	17.381
1600	31.669	150.482	111.066	63.065	-179.596	-115.267	15.745
1700	31.683	152.402	113.441	66.233	-179.409	-111.248	14.302
1800	31.695	154.214	115.657	69.402	-179.234	-107.248	13.021
1900	31.705	155.928	117.732	72.572	-179.072	-103.248	11.876
2000	31.714	157.554	119.683	75.743	-178.928	-99.264	10.847

*Data for crystal and liquid except enthalpy of formation at 298 K estimated.

Phase changes: 489.7 K, melting point of $TaCl_5$; $\Delta H° = 8.400$ kcal/mol.
506.9 K, boiling point of $TaCl_5$; $\Delta H° = 12.673$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-489.7 K: $Cp° = 35.350$

$H°- H°_{298} = 35.350\times10^{-3}T - 10.540$

489.7-506.9 K: $Cp° = 57.916 - 12.270\times10^{-3}T$

$H°- H°_{298} = 57.916\times10^{-3}T - 6.135\times10^{-6}T^2 - 11.719$

506.9-2000 K: $Cp° = 31.749 + 0.024\times10^{-3}T - 2.983\times10^{5}T^{-2}$

$H°- H°_{298} = 31.749\times10^{-3}T + 0.012\times10^{-6}T^2 + 2.983\times10^{2}T^{-1} + 12.050$

Formation equations (kcal/mol):

298.15-489.7 K: $\Delta Hf° = -207.278 + 8.226\times10^{-3}T - 0.902\times10^{-6}T^2 - 117.550T^{-1}$

$\Delta Gf° = -207.278 - 8.226\times10^{-3}T\ln T + 0.902\times10^{-6}T^2 - 58.775T^{-1} + 144.044\times10^{-3}T$

489.7-506.9 K: $\Delta Hf° = -208.458 + 30.793\times10^{-3}T - 7.037\times10^{-6}T^2 - 117.550T^{-1}$

$\Delta Gf° = -208.458 - 30.793\times10^{-3}T\ln T + 7.037\times10^{-6}T^2 - 58.775T^{-1} + 283.217\times10^{-3}T$

506.9-2000 K: $\Delta Hf° = -184.689 + 4.625\times10^{-3}T - 0.890\times10^{-6}T^2 + 180.750T^{-1}$

$\Delta Gf° = -184.689 - 4.625\times10^{-3}T\ln T + 0.890\times10^{-6}T^2 + 90.375T^{-1} + 75.885\times10^{-3}T$

Source: Data from Chase (26) who estimated data for crystal and liquid.

$TaCl_5(g)$

Tantalum Pentachloride (ideal gas)

[Formation: $Ta(c) + 2.5Cl_2(g) = TaCl_5(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	28.713	98.675	98.675	0	-182.800	-169.541	124.275
300	28.745	98.853	98.676	.053	-182.796	-169.458	123.449
400	29.953	107.309	99.821	2.995	-182.545	-165.052	90.179
500	30.575	114.066	102.016	6.025	-182.272	-160.707	70.244
600	30.931	119.675	104.505	9.102	-181.997	-156.420	56.975
700	31.153	124.461	107.022	12.207	-181.723	-152.179	47.512
800	31.300	128.631	109.468	15.330	-181.458	-147.979	40.425
900	31.401	132.324	111.807	18.465	-181.196	-143.809	34.921
1000	31.475	135.636	114.027	21.609	-180.941	-139.671	30.525
1100	31.530	138.639	116.130	24.760	-180.692	-135.555	26.932
1200	31.572	141.384	118.122	27.915	-180.453	-131.462	23.942
1300	31.604	143.913	120.010	31.074	-180.222	-127.389	21.416
1400	31.630	146.256	121.802	34.235	-180.002	-123.334	19.253
1500	31.651	148.439	123.506	37.399	-179.793	-119.294	17.381
1600	31.669	150.482	125.129	40.565	-179.596	-115.267	15.745
1700	31.683	152.402	126.677	43.733	-179.409	-111.248	14.302
1800	31.695	154.214	128.157	46.902	-179.234	-107.248	13.021
1900	31.705	155.928	129.574	50.072	-179.072	-103.248	11.876
2000	31.714	157.554	130.932	53.243	-178.928	-99.264	10.847

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 31.532 + 0.164\times10^{-3}T - 2.549\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 31.532\times10^{-3}T + 0.082\times10^{-6}T^2 + 2.549\times10^{2}T^{-1} - 10.263$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -184.502 + 4.409\times10^{-3}T - 0.820\times10^{-6}T^2 + 137.350T^{-1}$

$\Delta Gf^\circ = -184.502 - 4.409\times10^{-3}T\ln T + 0.820\times10^{-6}T^2 + 68.675T^{-1} + 74.280\times10^{-3}T$

Source: Data from Chase (26).

$TbBr_3(g)$

Terbium Tribromide (ideal gas)

[Formation: $Tb(c,l) + 1.5Br_2(l,g) = TbBr_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.105	96.159	96.159	0	-129.200	-136.377	99.965
300	19.114	96.277	96.160	.035	-129.227	-136.422	99.382
332.6	19.232	98.255	96.270	.660	-129.709	-137.179	90.138
332.6	19.232	98.255	96.270	.660	-140.307	-137.179	90.138
400	19.477	101.830	96.912	1.967	-140.343	-136.545	74.604
500	19.732	106.205	98.351	3.927	-140.386	-135.596	59.268
600	19.968	109.823	99.970	5.912	-140.429	-134.632	49.039
700	20.199	112.918	101.602	7.921	-140.493	-133.660	41.730
800	20.422	115.630	103.190	9.952	-140.572	-132.672	36.244
900	20.627	118.048	104.710	12.004	-140.669	-131.684	31.977
1000	20.808	120.231	106.155	14.076	-140.787	-130.685	28.561
1100	20.962	122.221	107.526	16.165	-140.926	-129.660	25.761
1200	21.087	124.051	108.828	18.268	-141.092	-128.634	23.427
1300	21.184	125.743	110.065	20.382	-141.294	-127.585	21.449
1400	21.255	127.315	111.241	22.504	-141.538	-126.515	19.750
1500	21.302	128.783	112.362	24.632	-141.830	-125.432	18.275
1560	21.318	129.619	113.010	25.910	-142.034	-124.778	17.481
1560	21.318	129.619	113.010	25.910	-143.234	-124.778	17.481
1600	21.328	130.159	113.432	26.763	-143.191	-124.301	16.979
1630	21.331	130.555	113.744	27.403	-143.161	-123.956	16.620
1630	21.331	130.555	113.744	27.403	-145.741	-123.956	16.620
1700	21.338	131.453	114.455	28.897	-145.982	-123.017	15.815
1800	21.333	132.672	115.433	31.031	-146.325	-121.662	14.772
1900	21.317	133.825	116.371	33.163	-146.672	-120.282	13.835
2000	21.293	134.918	117.271	35.294	-147.023	-118.886	12.991

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.
1560 K, α - β transition point of Tb; $\Delta H° = 1.200$ kcal/mol.
1630 K, melting point of Tb; $\Delta H° = 2.580$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.601 + 1.122\times10^{-3}T - 0.738\times10^{5}T^{-2}$

$H°- H°_{298} = 19.601\times10^{-3}T + 0.561\times10^{-6}T^2 + 0.738\times10^{2}T^{-1} - 6.141$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -126.206 - 11.819\times10^{-3}T - 1.403\times10^{-6}T^2 + 195.200T^{-1}$

$\Delta Gf° = -126.206 + 11.819\times10^{-3}T\ln T + 1.403\times10^{-6}T^2 + 97.600T^{-1} - 102.971\times10^{-3}T$

332.6-1560 K: $\Delta Hf° = -141.207 + 1.922\times10^{-3}T - 1.635\times10^{-6}T^2 + 148.100T^{-1}$

$\Delta Gf° = -141.207 - 1.922\times10^{-3}T\ln T + 1.635\times10^{-6}T^2 + 74.050T^{-1} + 22.061\times10^{-3}T$

1560-1630 K: $\Delta Hf° = -143.796 - 0.435\times10^{-3}T + 0.479\times10^{-6}T^2 + 26.700T^{-1}$

$\Delta Gf° = -143.796 + 0.435\times10^{-3}T\ln T - 0.479\times10^{-6}T^2 + 13.350T^{-1} + 9.714\times10^{-3}T$

1630-2000 K: $\Delta Hf° = -139.092 - 4.904\times10^{-3}T + 0.479\times10^{-6}T^2 + 26.700T^{-1}$

$\Delta Gf° = -139.092 + 4.904\times10^{-3}T\ln T - 0.479\times10^{-6}T^2 + 13.350T^{-1} - 26.226\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166) and Kim (122). Other data based on Myers (165) and Dieke (56).

$TbCl_3$(c,l)
Terbium Trichloride
[Formation: $Tb(c) + 1.5Cl_2(g) = TbCl_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	23.300	36.600	36.600	0	-238.300	-220.156	161.377
300	23.325	36.744	36.601	.043	-238.293	-220.045	160.300
400	24.430	43.613	37.530	2.433	-237.833	-214.031	116.939
500	25.317	49.162	39.318	4.922	-237.303	-208.142	90.978
600	26.117	53.850	41.360	7.494	-236.730	-202.363	73.710
700	26.875	57.933	43.442	10.144	-236.131	-196.681	61.406
783	27.487	60.978	45.142	12.400	-235.611	-192.030	53.598
783	29.860	65.276	45.142	15.765	-232.246	-192.030	53.598
800	29.860	65.917	45.576	16.273	-232.098	-191.158	52.221
855	29.860	67.902	46.949	17.915	-231.625	-188.360	48.147
855	34.530	73.311	46.949	22.540	-227.000	-188.360	48.147
900	34.530	75.083	48.312	24.094	-226.413	-186.342	45.249
1000	34.530	78.721	51.174	27.547	-225.141	-181.965	39.768
1100	34.530	82.012	53.830	31.000	-223.908	-177.700	35.305
1200	34.530	85.017	56.306	34.453	-222.719	-173.559	31.609
1300	34.530	87.781	58.623	37.906	-221.578	-169.505	28.496

*Entropy and heat capacity at 298 K estimated.

Phase changes: 783 K, α - β transition point of $TbCl_3$; ΔH° = 3.365 kcal/mol.
855 K, melting point of $TbCl_3$; ΔH° = 4.625 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-783 K: $Cp^\circ = 22.159 + 6.980\times10^{-3}T - 0.836\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 22.159\times10^{-3}T + 3.490\times10^{-6}T^2 + 0.836\times10^{2}T^{-1} - 7.197$

783-855 K: $Cp^\circ = 29.860$
$H^\circ - H^\circ_{298} = 29.860\times10^{-3}T - 7.615$

855-1300 K: $Cp^\circ = 34.530$
$H^\circ - H^\circ_{298} = 34.530\times10^{-3}T - 6.983$

Formation equations (kcal/mol):

298.15-783 K: $\Delta Hf^\circ = -240.136 + 4.635\times10^{-3}T + 1.244\times10^{-6}T^2 + 102.550T^{-1}$
$\Delta Gf^\circ = -240.136 - 4.635\times10^{-3}T\ln T - 1.244\times10^{-6}T^2 + 51.275T^{-1} + 93.214\times10^{-3}T$

783-855 K: $\Delta Hf^\circ = -240.555 + 12.336\times10^{-3}T - 2.246\times10^{-6}T^2 + 18.950T^{-1}$
$\Delta Gf^\circ = -240.555 - 12.336\times10^{-3}T\ln T + 2.246\times10^{-6}T^2 + 9.475T^{-1} + 142.396\times10^{-3}T$

855-1300 K: $\Delta Hf^\circ = -239.923 + 17.005\times10^{-3}T - 2.246\times10^{-6}T^2 + 18.950T^{-1}$
$\Delta Gf^\circ = -239.923 - 17.005\times10^{-3}T\ln T + 2.246\times10^{-6}T^2 + 9.475T^{-1} + 173.185\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (207). Entropy and heat capacity at 298 K estimated. High-temperature data based on Dworkin (69).

$TbCl_3(g)$

Terbium Trichloride (ideal gas)

[Formation: $Tb(c,l) + 1.5Cl_2(g) = TbCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.695	89.681	89.681	0	-165.200	-162.882	119.394
300	18.708	89.797	89.681	.035	-165.201	-162.869	118.648
400	19.229	95.258	90.423	1.934	-165.231	-162.088	88.559
500	19.567	99.586	91.836	3.875	-165.250	-161.301	70.504
600	19.851	103.179	93.436	5.846	-165.279	-160.508	58.464
700	20.112	106.259	95.053	7.844	-165.331	-159.710	49.863
800	20.354	108.961	96.627	9.867	-165.403	-158.899	43.409
900	20.573	111.371	98.133	11.914	-165.492	-158.081	38.387
1000	20.765	113.549	99.568	13.981	-165.606	-157.258	34.368
1100	20.926	115.536	100.931	16.066	-165.742	-156.410	31.075
1200	21.057	117.362	102.225	18.165	-165.907	-155.561	28.331
1300	21.158	119.052	103.455	20.276	-166.108	-154.687	26.005
1400	21.232	120.623	104.626	22.396	-166.351	-153.794	24.008
1500	21.282	122.090	105.742	24.522	-166.642	-152.888	22.275
1560	21.299	122.925	106.386	25.800	-166.845	-152.339	21.342
1560	21.299	122.925	106.386	25.800	-168.045	-152.339	21.342
1600	21.311	123.464	106.806	26.652	-168.003	-151.932	20.753
1630	21.314	123.860	107.117	27.291	-167.973	-151.640	20.332
1630	21.314	123.860	107.117	27.291	-170.553	-151.640	20.332
1700	21.322	124.756	107.824	28.784	-170.795	-150.819	19.389
1800	21.319	125.975	108.799	30.916	-171.139	-149.644	18.169
1900	21.305	127.128	109.735	33.047	-171.487	-148.441	17.074
2000	21.282	128.220	110.632	35.177	-171.840	-147.218	16.087

Phase changes: 1560 K, α - β transition point of Tb; $\Delta H° = 1.200$ kcal/mol.
1630 K, melting point of Tb; $\Delta H° = 2.580$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.568 + 1.140\times10^{-3}T - 1.078\times10^{5}T^{-2}$

$H°- H°_{298} = 19.568\times10^{-3}T + 0.570\times10^{-6}T^{2} + 1.078\times10^{2}T^{-1} - 6.246$

Formation equations (kcal/mol):

298.15-1560 K: $\Delta Hf° = -166.085 + 2.044\times10^{-3}T - 1.676\times10^{-6}T^{2} + 126.750T^{-1}$

$\Delta Gf° = -166.085 - 2.044\times10^{-3}T\ln T + 1.676\times10^{-6}T^{2} + 63.375T^{-1} + 21.174\times10^{-3}T$

1560-1630 K: $\Delta Hf° = -168.675 - 0.313\times10^{-3}T + 0.438\times10^{-6}T^{2} + 5.350T^{-1}$

$\Delta Gf° = -168.675 + 0.313\times10^{-3}T\ln T - 0.438\times10^{-6}T^{2} + 2.675T^{-1} + 8.827\times10^{-3}T$

1630-2000 K: $\Delta Hf° = -163.971 - 4.782\times10^{-3}T + 0.438\times10^{-6}T^{2} + 5.350T^{-1}$

$\Delta Gf° = -163.971 + 4.782\times10^{-3}T\ln T - 0.438\times10^{-6}T^{2} + 2.675T^{-1} - 27.113\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (167). Other data based on Myers (165) and Dieke (56).

TbF_3(c,l)
Terbium Trifluoride
[Formation: $Tb(c,l) + 1.5F_2(g) = TbF_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	21.800	28.200	28.200	0	-408.000	-389.519	285.522
300	21.836	28.335	28.202	.040	-407.994	-389.406	283.679
400	23.422	34.851	29.079	2.309	-407.564	-383.272	209.407
500	24.535	40.203	30.783	4.710	-407.049	-377.260	164.898
600	25.407	44.756	32.743	7.208	-406.491	-371.355	135.264
700	26.128	48.728	34.748	9.786	-405.918	-365.542	114.126
800	26.746	52.259	36.720	12.431	-405.333	-359.810	98.294
900	27.295	55.441	38.627	15.133	-404.739	-354.157	86.000
1000	27.802	58.343	40.455	17.888	-404.144	-348.575	76.180
1100	28.291	61.016	42.204	20.693	-403.543	-343.039	68.155
1200	28.785	63.499	43.877	23.546	-402.941	-337.572	61.480
1300	29.305	65.823	45.476	26.451	-402.337	-332.144	55.838
1400	29.870	68.015	47.009	29.409	-401.736	-326.763	51.009
1450	30.177	69.069	47.752	30.910	-401.434	-324.091	48.848
1450	36.300	78.717	47.751	44.900	-387.444	-324.091	48.848
1500	36.300	79.948	48.805	46.715	-386.842	-321.917	46.903
1560	36.300	81.371	50.029	48.893	-386.143	-319.338	44.737
1560	36.300	81.371	50.029	48.893	-387.343	-319.338	44.737
1600	36.300	82.290	50.824	50.345	-386.701	-317.598	43.381
1630	36.300	82.964	51.410	51.434	-386.220	-316.316	42.411
1630	36.300	82.964	51.410	51.434	-388.800	-316.316	42.411
1700	36.300	84.491	52.741	53.975	-387.992	-313.219	40.266
1800	36.300	86.566	54.563	57.605	-386.840	-308.863	37.501
1900	36.300	88.529	56.300	61.235	-385.691	-304.563	35.032
2000	36.300	90.391	57.958	64.865	-384.548	-300.324	32.817

*Entropy and heat capacity at 298 K estimated.

Phase changes: 1450 K, melting point of TbF_3; ΔH° = 13.990 kcal/mol.
1560 K, α - β transition point of Tb; ΔH° = 1.200 kcal/mol.
1630 K, melting point of Tb; ΔH° = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1450 K: $Cp^\circ = 23.091 + 4.934\times10^{-3}T - 2.456\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 23.091\times10^{-3}T + 2.467\times10^{-6}T^2 + 2.456\times10^{2}T^{-1} - 7.928$
1450-2000 K: $Cp^\circ = 36.300$
$H^\circ - H^\circ_{298} = 36.300\times10^{-3}T - 7.735$

Formation equations (kcal/mol):

298.15-1450 K: $\Delta Hf^\circ = -410.536 + 6.045\times10^{-3}T + 0.092\times10^{-6}T^2 + 216.250T^{-1}$
$\Delta Gf^\circ = -410.536 - 6.045\times10^{-3}T\ln T - 0.092\times10^{-6}T^2 + 108.125T^{-1} + 103.743\times10^{-3}T$
1450-1560 K: $\Delta Hf^\circ = -410.343 + 19.254\times10^{-3}T - 2.375\times10^{-6}T^2 - 29.350T^{-1}$
$\Delta Gf^\circ = -410.343 - 19.254\times10^{-3}T\ln T + 2.375\times10^{-6}T^2 - 14.675T^{-1} + 196.243\times10^{-3}T$
1560-1630 K: $\Delta Hf^\circ = -412.933 + 16.897\times10^{-3}T - 0.261\times10^{-6}T^2 - 150.750T^{-1}$
$\Delta Gf^\circ = -412.933 - 16.897\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 - 75.375T^{-1} + 183.896\times10^{-3}T$
1630-2000 K: $\Delta Hf^\circ = -408.228 + 12.428\times10^{-3}T - 0.261\times10^{-6}T^2 - 150.750T^{-1}$
$\Delta Gf^\circ = -408.228 - 12.428\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 - 75.375T^{-1} + 147.956\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Kim (122). Entropy and heat capacity at 298 K estimated. High-temperature data based on Spedding (222).

$TbF_3(g)$

Terbium Trifluoride (ideal gas)

[Formation: $Tb(c,l) + 1.5F_2(g) = TbF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	17.090	81.179	81.179	0	-301.500	-298.815	219.034
300	17.115	81.284	81.179	.032	-301.502	-298.799	217.672
400	18.152	86.363	81.866	1.799	-301.573	-297.887	162.756
500	18.813	90.489	83.189	3.650	-301.609	-296.963	129.801
600	19.301	93.964	84.704	5.556	-301.643	-296.031	107.828
700	19.696	96.970	86.246	7.507	-301.698	-295.091	92.130
800	20.029	99.622	87.755	9.494	-301.771	-294.138	80.354
900	20.313	101.998	89.208	11.511	-301.861	-293.180	71.193
1000	20.552	104.151	90.596	13.555	-301.977	-292.216	63.863
1100	20.749	106.119	91.919	15.620	-302.116	-291.225	57.860
1200	20.907	107.932	93.179	17.703	-302.284	-290.235	52.858
1300	21.030	109.610	94.379	19.800	-302.488	-289.218	48.621
1400	21.121	111.172	95.523	21.908	-302.737	-288.184	44.987
1500	21.185	112.632	96.616	24.024	-303.034	-287.134	41.835
1560	21.210	113.464	97.249	25.295	-303.241	-286.500	40.137
1560	21.210	113.464	97.249	25.295	-304.441	-286.500	40.137
1600	21.226	114.001	97.661	26.144	-304.401	-286.037	39.070
1630	21.232	114.395	97.965	26.781	-304.373	-285.701	38.306
1630	21.232	114.395	97.965	26.781	-306.953	-285.701	38.306
1700	21.247	115.288	98.660	28.268	-307.199	-284.781	36.611
1800	21.252	116.503	99.618	30.393	-307.552	-283.461	34.416
1900	21.244	117.652	100.537	32.518	-307.908	-282.114	32.450
2000	21.227	118.741	101.420	34.642	-308.271	-280.746	30.678

Phase changes: 1560 K, α - β transition point of Tb; $\Delta H° = 1.200$ kcal/mol.
1630 K, melting point of Tb; $\Delta H° = 2.580$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.246 + 1.324\times10^{-3}T - 2.268\times10^{5}T^{-2}$

$H°- H°_{298} = 19.246\times10^{-3}T + 0.662\times10^{-6}T^2 + 2.268\times10^{2}T^{-1} - 6.558$

Formation equations (kcal/mol):

298.15-1560 K: $\Delta Hf° = -302.666 + 2.200\times10^{-3}T - 1.713\times10^{-6}T^2 + 197.450T^{-1}$

$\Delta Gf° = -302.666 - 2.200\times10^{-3}T\ln T + 1.713\times10^{-6}T^2 + 98.725T^{-1} + 23.829\times10^{-3}T$

1560-1630 K: $\Delta Hf° = -305.256 - 0.157\times10^{-3}T + 0.401\times10^{-6}T^2 + 76.050T^{-1}$

$\Delta Gf° = -305.256 + 0.157\times10^{-3}T\ln T - 0.401\times10^{-6}T^2 + 38.025T^{-1} + 11.483\times10^{-3}T$

1630-2000 K: $\Delta Hf° = -300.551 - 4.626\times10^{-3}T + 0.401\times10^{-6}T^2 + 76.050T^{-1}$

$\Delta Gf° = -300.551 + 4.626\times10^{-3}T\ln T - 0.401\times10^{-6}T^2 + 38.025T^{-1} - 24.458\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

TbI_3(c,l)
Terbium Triiodide
[Formation: $Tb(c) + 1.5I_2(c,l,g) = TbI_3(c,l)$

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	23.400	54.900	54.900	0	-145.000	-143.731	105.356
300	23.429	55.045	54.902	.043	-145.006	-143.724	104.701
386.8	24.641	61.155	55.642	2.133	-145.323	-143.315	80.975
386.8	24.641	61.155	55.642	2.133	-150.887	-143.315	80.975
400	24.825	61.985	55.838	2.459	-151.033	-143.054	78.160
458.4	25.294	65.411	56.843	3.928	-151.650	-141.845	67.626
458.4	25.294	65.411	56.843	3.928	-166.681	-141.845	67.626
500	25.628	67.623	57.649	4.987	-166.462	-139.599	61.018
600	25.885	72.325	59.715	7.566	-165.924	-134.277	48.910
700	25.922	76.318	61.808	10.157	-165.415	-129.042	40.288
800	26.144	79.790	63.844	12.757	-164.934	-123.873	33.840
900	26.988	82.909	65.791	15.406	-164.441	-118.773	28.842
1000	28.906	85.841	67.651	18.190	-163.855	-113.733	24.856
1080	31.519	88.157	69.083	20.600	-163.230	-109.740	22.207
1080	29.730	88.324	69.083	20.780	-163.050	-109.740	22.207
1100	29.730	88.870	69.438	21.375	-162.906	-108.754	21.607
1200	29.730	91.456	71.166	24.348	-162.210	-103.867	18.917
1228	29.730	92.142	71.637	25.180	-162.024	-102.509	18.244
1228	37.600	103.323	71.637	38.910	-148.294	-102.509	18.244
1300	37.600	105.465	73.452	41.617	-147.264	-99.850	16.786

*Data at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
1080 K, α - β transition point of TbI_3; ΔH° = 0.180 kcal/mol.
1228 K, melting point of TbI_3; ΔH° = 13.730 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1080 K: $Cp^\circ = 22.373 + 6.084\times10^{-3}T - 0.701\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 22.373\times10^{-3}T + 3.042\times10^{-6}T^2 + 0.701\times10^{2}T^{-1} - 7.176$
1080-1228 K: $Cp^\circ = 29.730$
$H^\circ - H^\circ_{298} = 29.730\times10^{-3}T - 11.328$
1228-1300 K: $Cp^\circ = 37.600$
$H^\circ - H^\circ_{298} = 37.600\times10^{-3}T - 7.263$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -145.160 - 1.227\times10^{-3}T - 1.310\times10^{-6}T^2 + 191.500T^{-1}$
$\Delta Gf^\circ = -145.160 + 1.227\times10^{-3}T\ln T + 1.310\times10^{-6}T^2 + 95.750T^{-1} - 3.662\times10^{-3}T$
386.8-458.4 K: $\Delta Hf^\circ = -147.343 - 10.833\times10^{-3}T + 0.928\times10^{-6}T^2 + 191.500T^{-1}$
$\Delta Gf^\circ = -147.343 + 10.833\times10^{-3}T\ln T - 0.928\times10^{-6}T^2 + 95.750T^{-1} - 54.385\times10^{-3}T$
458.4-1080 K: $\Delta Hf^\circ = -169.413 + 4.677\times10^{-3}T + 0.826\times10^{-6}T^2 + 168.550T^{-1}$
$\Delta Gf^\circ = -169.413 - 4.677\times10^{-3}T\ln T - 0.826\times10^{-6}T^2 + 84.275T^{-1} + 88.810\times10^{-3}T$
1080-1228 K: $\Delta Hf^\circ = -173.565 + 12.035\times10^{-3}T - 2.216\times10^{-6}T^2 + 98.450T^{-3}$
$\Delta Gf^\circ = -173.565 - 12.035\times10^{-3}T\ln T + 2.216\times10^{-6}T^2 + 49.225T^{-1} + 140.786\times10^{-3}T$
1228-1300 K: $\Delta Hf^\circ = -169.500 + 19.904\times10^{-3}T - 2.216\times10^{-6}T^2 + 98.450T^{-1}$
$\Delta Gf^\circ = -169.500 - 19.904\times10^{-3}T\ln T + 2.216\times10^{-6}T^2 + 49.225T^{-1} + 193.456\times10^{-3}T$

Sources: Enthalpy of formation at 298 K estimated by Kim (122). Entropy and heat capacity at 298 K estimated. High-temperature data based on Dworkin (69).

$TbI_3(g)$

Terbium Triiodide (ideal gas)

[Formation: $Tb(c,l) + 1.5I_2(c,l,g) = TbI_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.479	102.994	102.994	0	-79.600	-92.670	67.928
300	19.485	103.114	102.994	.036	-79.613	-92.752	67.569
386.8	19.667	108.090	103.601	1.736	-80.320	-96.465	54.504
386.8	19.667	108.090	103.601	1.736	-85.883	-96.465	54.504
400	19.695	108.750	103.760	1.996	-86.096	-96.823	52.901
458.4	19.800	111.441	104.572	3.149	-87.029	-98.324	46.877
458.4	19.800	111.441	104.572	3.149	-102.061	-98.324	46.877
500	19.875	113.164	105.216	3.974	-102.075	-97.982	42.827
600	20.068	116.805	106.853	5.971	-102.119	-97.160	35.390
700	20.274	119.914	108.503	7.988	-102.184	-96.328	30.075
800	20.479	122.634	110.102	10.026	-102.264	-95.479	26.083
900	20.672	125.058	111.631	12.084	-102.364	-94.629	22.979
1000	20.845	127.245	113.085	14.160	-102.485	-93.768	20.493
1100	20.993	129.239	114.464	16.252	-102.629	-92.883	18.454
1200	21.113	131.071	115.773	18.357	-102.801	-91.996	16.755
1300	21.206	132.765	117.017	20.473	-103.007	-91.084	15.312
1400	21.274	134.339	118.198	22.598	-103.257	-90.151	14.073
1500	21.318	135.808	119.323	24.727	-103.556	-89.206	12.997
1560	21.333	136.645	119.973	26.007	-103.762	-88.631	12.417
1560	21.333	136.645	119.973	26.007	-104.962	-88.631	12.417
1600	21.343	137.185	120.397	26.861	-104.922	-88.208	12.049
1630	21.345	137.581	120.710	27.501	-104.894	-87.904	11.786
1630	21.345	137.581	120.710	27.501	-107.474	-87.904	11.786
1700	21.350	138.479	121.423	28.995	-107.722	-87.059	11.192
1800	21.344	139.699	122.405	31.130	-108.073	-85.842	10.422
1900	21.328	140.853	123.346	33.264	-108.428	-84.598	9.731
2000	21.302	141.946	124.248	35.395	-108.788	-83.334	9.106

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
1560 K, α - β transition point of Tb; $\Delta H°$ = 1.200 kcal/mol.
1630 K, melting point of Tb; $\Delta H°$ = 2.580 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.620 + 1.110\times10^{-3}T - 0.420\times10^{5}T^{-2}$

$H°- H°_{298} = 19.620\times10^{-3}T + 0.555\times10^{-6}T^{2} + 0.420\times10^{2}T^{-1} - 6.040$

$TbI_3(g)$ - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -78.624 - 3.979\times10^{-3}T - 3.797\times10^{-6}T^2 + 163.400T^{-1}$

$\Delta Gf^\circ = -78.624 + 3.979\times10^{-3}T\ln T + 3.797\times10^{-6}T^2 + 81.700T^{-1} - 71.835\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -80.807 - 13.586\times10^{-3}T - 1.559\times10^{-6}T^2 + 163.400T^{-1}$

$\Delta Gf^\circ = -80.807 + 13.586\times10^{-3}T\ln T + 1.559\times10^{-6}T^2 + 81.700T^{-1} - 122.558\times10^{-3}T$

458.4-1560 K: $\Delta Hf^\circ = -102.877 + 1.925\times10^{-3}T - 1.661\times10^{-6}T^2 + 140.450T^{-1}$

$\Delta Gf^\circ = -102.877 - 1.925\times10^{-3}T\ln T + 1.661\times10^{-6}T^2 + 70.225T^{-1} + 20.636\times10^{-3}T$

1560-1630 K: $\Delta Hf^\circ = -105.466 - 0.432\times10^{-3}T + 0.453\times10^{-6}T^2 + 19.050T^{-1}$

$\Delta Gf^\circ = -105.466 + 0.432\times10^{-3}T\ln T - 0.453\times10^{-6}T^2 + 9.525T^{-1} + 8.290\times10^{-3}T$

1630-2000 K: $\Delta Hf^\circ = -100.762 - 4.901\times10^{-3}T + 0.453\times10^{-6}T^2 + 19.050T^{-1}$

$\Delta Gf^\circ = -100.762 + 4.901\times10^{-3}T\ln T - 0.453\times10^{-6}T^2 + 9.525T^{-1} - 27.651\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

$TeCl_2(g)$

Tellurium Dichloride (ideal gas)

[Reaction: $0.5Te_2(g) + Cl_2(g) = TeCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	12.990	73.030	73.030	0	-46.165	-42.827	31.393
300	13.000	73.110	73.030	.024	-46.164	-42.807	31.184
400	13.390	76.920	73.552	1.347	-46.111	-41.699	22.783
500	13.560	79.930	74.538	2.696	-46.063	-40.601	17.746
600	13.660	82.410	75.647	4.058	-46.026	-39.508	14.391
700	13.720	84.520	76.767	5.427	-46.000	-38.425	11.997
800	13.760	86.350	77.847	6.802	-45.984	-37.341	10.201
900	13.790	87.980	78.891	8.180	-45.976	-36.268	8.807
1000	13.810	89.430	79.870	9.560	-45.979	-35.186	7.690
1100	13.830	90.750	80.803	10.942	-45.991	-34.107	6.776
1200	13.840	91.950	81.679	12.325	-46.013	-33.021	6.014
1300	13.850	93.060	82.514	13.710	-46.042	-31.940	5.369
1400	13.860	94.090	83.308	15.095	-46.082	-30.859	4.817
1500	13.870	95.040	84.052	16.482	-46.123	-29.761	4.336
1600	13.870	95.940	84.772	17.869	-46.166	-28.680	3.917
1700	13.880	96.780	85.453	19.256	-46.209	-27.575	3.545
1800	13.880	97.570	86.101	20.645	-46.250	-26.476	3.215
1900	13.890	98.320	86.724	22.033	-46.292	-25.373	2.919
2000	13.890	99.040	87.329	23.422	-46.333	-24.285	2.654

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.877 + 0.016\times10^{-3}T - 0.793\times10^{5}T^{-2}$

$H°- H°_{298} = 13.877\times10^{-3}T + 0.008\times10^{-6}T^{2} + 0.793\times10^{2}T^{-1} - 4.404$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr° = -46.352 + 0.750\times10^{-3}T - 0.377\times10^{-6}T^{2} - 1.100T^{-1}$

$\Delta Gr° = -46.352 - 0.750\times10^{-3}T\ln T + 0.377\times10^{-6}T^{2} - 0.550T^{-1} + 15.991\times10^{-3}T$

Source: Data from Mills (159).

$TeCl_4(c,l)$

Tellurium Tetrachloride

[Reaction: $0.5Te_2(g) + 2Cl_2(g) = TeCl_4(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15*	33.100	48.000	48.000	0	-96.565	-69.876	51.220
300	33.100	48.200	48.000	.061	-96.542	-69.710	50.783
400	33.100	57.740	49.300	3.376	-95.327	-60.953	33.302
497	33.100	64.930	51.676	6.586	-94.205	-52.743	23.193
497	55.000	74.000	51.676	11.096	-89.695	-52.743	23.193
500	55.000	74.340	51.818	11.261	-89.596	-52.524	22.958
600	55.000	84.360	56.425	16.761	-86.290	-45.414	16.542
700	55.000	92.840	61.039	22.261	-83.011	-38.864	12.134

*Entropy at 298 K estimated.

Phase changes: 497 K, melting point of $TeCl_4$; $\Delta H°$ = 4.510 kcal/mol.
689 K, boiling point of $TeCl_4$; $\Delta H°$ vaporization at 298 K = 28 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-497 K: $Cp° = 33.118$

$H°- H°_{298} = 33.118\times10^{-3}T - 9.874$

497-700 K: $Cp° = 55.000$

$H°- H°_{298} = 55.000\times10^{-3}T - 16.239$

Reaction equations (kcal/mol):

298.15-497 K: $\Delta Hr° = -99.353 + 11.164\times10^{-3}T - 0.472\times10^{-6}T^2 - 148.700T^{-1}$

$\Delta Gr° = -99.353 - 11.164\times10^{-3}T\ln T + 0.472\times10^{-6}T^2 - 74.350T^{-1} + 163.172\times10^{-3}T$

497-700 K: $\Delta Hr° = -105.718 + 33.046\times10^{-3}T - 0.472\times10^{-6}T^2 - 148.700T^{-1}$

$\Delta Gr° = -105.718 - 33.046\times10^{-3}T\ln T + 0.472\times10^{-6}T^2 - 74.350T^{-1} + 311.836\times10^{-3}T$

Source: Data from Mills (159) who estimated entropy at 298 K.

TeF(g)
Tellurium Monofluoride (ideal gas)
[Reaction: $0.5Te_2(g) + 0.5F_2(g) = TeF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15*	7.930	57.660	57.660	0	-39.965	-40.711	29.842
300	7.940	57.710	57.660	.015	-39.965	-40.717	29.662
400	8.330	60.060	57.980	.832	-39.972	-40.966	22.382
500	8.510	61.940	58.590	1.675	-39.979	-41.213	18.014
600	8.620	63.500	59.282	2.531	-39.994	-41.457	15.101
700	8.680	64.830	59.979	3.396	-40.018	-41.697	13.018
800	8.730	66.000	60.666	4.267	-40.051	-41.942	11.458
900	8.760	67.030	61.317	5.142	-40.092	-42.176	10.242
1000	8.790	67.950	61.931	6.019	-40.144	-42.401	9.267
1100	8.810	68.790	62.518	6.899	-40.204	-42.624	8.468
1200	8.830	69.560	63.076	7.781	-40.272	-42.843	7.803
1300	8.850	70.270	63.605	8.665	-40.348	-43.057	7.238
1400	8.860	70.920	64.098	9.551	-40.433	-43.255	6.752
1500	8.880	71.530	64.571	10.438	-40.520	-43.451	6.331
1600	8.890	72.110	65.031	11.326	-40.606	-43.658	5.963
1700	8.900	72.650	65.464	12.216	-40.692	-43.839	5.636
1800	8.920	73.160	65.878	13.107	-40.776	-44.027	5.346
1900	8.930	73.640	66.272	13.999	-40.858	-44.200	5.084
2000	8.940	74.100	66.654	14.892	-40.939	-44.376	4.849

*Data estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.785 + 0.084\times10^{-3}T - 0.782\times10^{5}T^{-2}$

$H°- H°_{298} = 8.785\times10^{-3}T + 0.042\times10^{-6}T^{2} + 0.782\times10^{2}T^{-1} - 2.885$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr° = -40.057 + 0.231\times10^{-3}T - 0.341\times10^{-6}T^{2} + 15.850T^{-1}$

$\Delta Gr° = -40.057 - 0.231\times10^{-3}T\ln T + 0.341\times10^{-6}T^{2} + 7.925T^{-1} - 1.067\times10^{-3}T$

Source: Data are estimations from Mills (159).

$TeF_2(g)$

Tellurium Difluoride (ideal gas)

[Reaction: $0.5Te_2(g) + F_2(g) = TeF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15*	10.970	65.750	65.750	0	-111.165	-107.102	78.507
300	10.990	65.820	65.750	.021	-111.166	-107.077	78.005
400	12.120	69.160	66.195	1.186	-111.210	-105.704	57.753
500	12.650	71.930	67.076	2.427	-111.220	-104.326	45.600
600	12.950	74.270	68.088	3.709	-111.225	-102.948	37.498
700	13.140	76.280	69.117	5.014	-111.232	-101.568	31.710
800	13.280	78.040	70.121	6.335	-111.247	-100.185	27.369
900	13.380	79.610	71.090	7.668	-111.265	-98.801	23.992
1000	13.450	81.030	72.020	9.010	-111.292	-97.422	21.291
1100	13.520	82.310	72.893	10.359	-111.326	-96.024	19.078
1200	13.570	83.490	73.729	11.713	-111.368	-94.633	17.235
1300	13.620	84.580	74.524	13.073	-111.415	-93.238	15.675
1400	13.670	85.590	75.277	14.438	-111.471	-91.838	14.336
1500	13.710	86.540	76.003	15.806	-111.528	-90.444	13.178
1600	13.740	87.420	76.683	17.179	-111.583	-89.029	12.161
1700	13.780	88.260	77.345	18.555	-111.636	-87.620	11.264
1800	13.810	89.040	77.965	19.935	-111.688	-86.194	10.465
1900	13.850	89.790	78.570	21.318	-111.735	-84.780	9.752
2000	13.880	90.500	79.148	22.704	-111.781	-83.357	9.109

*Data estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.430 + 0.252\times10^{-3}T - 2.253\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.430\times10^{-3}T + 0.126\times10^{-6}T^2 + 2.253\times10^{2}T^{-1} - 4.771$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr^\circ = -111.698 + 0.622\times10^{-3}T - 0.345\times10^{-6}T^2 + 112.700T^{-1}$

$\Delta Gr^\circ = -111.698 - 0.622\times10^{-3}T\ln T + 0.345\times10^{-6}T^2 + 56.350T^{-1} + 18.226\times10^{-3}T$

Source: Data are estimations from Mills (159).

$TeF_4(g)$

Tellurium Tetrafluoride (ideal gas)

[Reaction: $0.5Te_2(g) + 2F_2(g) = TeF_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15*	19.620	77.460	77.460	0	-245.765	-230.750	169.142
300	19.670	77.590	77.460	.039	-245.762	-230.658	168.032
400	22.080	83.630	78.270	2.144	-245.635	-225.637	123.280
500	23.210	88.690	79.860	4.415	-245.420	-220.659	96.449
600	23.850	92.990	81.707	6.770	-245.181	-215.733	78.580
700	24.250	96.700	83.590	9.177	-244.935	-210.845	65.828
800	24.530	99.950	85.429	11.617	-244.691	-205.988	56.273
900	24.740	102.860	87.213	14.082	-244.449	-201.170	48.850
1000	24.900	105.470	88.906	16.564	-244.216	-196.371	42.916
1100	25.040	107.850	90.521	19.062	-243.987	-191.594	38.066
1200	25.150	110.040	92.064	21.571	-243.765	-186.849	34.029
1300	25.250	112.050	93.518	24.091	-243.547	-182.104	30.614
1400	25.340	113.930	94.915	26.621	-243.338	-177.396	27.692
1500	25.420	115.680	96.241	29.159	-243.128	-172.692	25.161
1600	25.500	117.320	97.504	31.705	-242.916	-168.001	22.948
1700	25.570	118.870	98.718	34.258	-242.700	-163.320	20.996
1800	25.630	120.330	99.876	36.818	-242.484	-158.656	19.263
1900	25.700	121.720	100.992	39.384	-242.261	-154.008	17.715
2000	25.760	123.040	102.061	41.958	-242.036	-149.368	16.322

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 24.908 + 0.482\times10^{-3}T - 4.829\times10^{5}T^{-2}$

$H°- H°_{298} = 24.908\times10^{-3}T + 0.241\times10^{-6}T^{2} + 4.829\times10^{2}T^{-1} - 9.067$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr° = -247.705 + 3.592\times10^{-3}T - 0.403\times10^{-6}T^{2} + 269.800T^{-1}$

$\Delta Gr° = -247.705 - 3.592\times10^{-3}T\ln T + 0.403\times10^{-6}T^{2} + 134.900T^{-1} + 75.699\times10^{-3}T$

Source: Data from Mills (159). All are estimates except enthalpy of formation at 298 K.

$TeF_5(g)$

Tellurium Pentafluoride (ideal gas)

[Reaction: $0.5Te_2(g) + 2.5F_2(g) = TeF_5(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15*	24.030	81.450	81.450	0	-296.365	-275.318	201.811
300	24.090	81.610	81.453	.047	-296.361	-275.189	200.473
400	27.130	89.020	82.442	2.631	-296.139	-268.157	146.512
500	28.550	95.250	84.406	5.422	-295.806	-261.202	114.170
600	29.340	100.530	86.663	8.320	-295.440	-254.314	92.633
700	29.850	105.090	88.974	11.281	-295.063	-247.488	77.268
800	30.200	109.100	91.244	14.285	-294.687	-240.719	65.761
900	30.450	112.670	93.428	17.318	-294.312	-233.992	56.820
1000	30.660	115.890	95.516	20.374	-293.945	-227.313	49.678
1100	30.820	118.820	97.504	23.448	-293.583	-220.664	43.841
1200	30.960	121.510	99.396	26.537	-293.226	-214.053	38.984
1300	31.080	123.990	101.191	29.639	-292.874	-207.464	34.877
1400	31.190	126.300	102.905	32.753	-292.531	-200.915	31.364
1500	31.290	128.460	104.542	35.877	-292.187	-194.390	28.322
1600	31.380	130.480	106.099	39.010	-291.841	-187.881	25.663
1700	31.470	132.380	107.585	42.152	-291.490	-181.376	23.317
1800	31.550	134.180	109.012	45.303	-291.138	-174.912	21.237
1900	31.630	135.890	110.384	48.462	-290.779	-168.466	19.378
2000	31.700	137.510	111.696	51.628	-290.421	-162.030	17.706

*Data estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 30.697 + 0.572\times10^{-3}T - 6.078\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 30.697\times10^{-3}T + 0.286\times10^{-6}T^2 + 6.078\times10^{2}T^{-1} - 11.216$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr^\circ = -299.009 + 5.127\times10^{-3}T - 0.446\times10^{-6}T^2 + 344.450T^{-1}$

$\Delta Gr^\circ = -299.009 - 5.127\times10^{-3}T\ln T + 0.446\times10^{-6}T^2 + 172.225T^{-1} + 106.606\times10^{-3}T$

Source: Data are estimations from Mills (159).

$TeF_6(g)$

Tellurium Hexafluoride (ideal gas)

[Reaction: $0.5Te_2(g) + 3F_2(g) = TeF_6(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHr°	ΔGr°	
298.15	28.030	80.280	80.280	0	-346.365	-317.747	232.912
300	28.100	80.470	80.283	.056	-346.359	-317.572	231.348
400	31.910	89.160	81.448	3.085	-346.077	-308.011	168.287
500	33.690	96.490	83.742	6.374	-345.648	-298.541	130.490
600	34.690	102.730	86.403	9.796	-345.172	-289.165	105.327
700	35.320	108.120	89.121	13.299	-344.677	-279.864	87.376
800	35.760	112.870	91.803	16.854	-344.182	-270.645	73.936
900	36.080	117.100	94.382	20.446	-343.683	-261.480	63.495
1000	36.330	120.920	96.853	24.067	-343.191	-252.381	55.157
1100	36.540	124.390	99.198	27.711	-342.702	-243.317	48.342
1200	36.710	127.570	101.426	31.373	-342.218	-234.296	42.670
1300	36.860	130.520	103.557	35.052	-341.736	-225.326	37.880
1400	37.000	133.260	105.585	38.745	-341.264	-216.399	33.781
1500	37.120	135.810	107.509	42.451	-340.789	-207.487	30.230
1600	37.240	138.210	109.354	46.169	-340.311	-198.618	27.130
1700	37.340	140.470	111.118	49.898	-339.827	-189.766	24.396
1800	37.450	142.610	112.811	53.638	-339.343	-180.962	21.972
1900	37.540	144.640	114.436	57.387	-338.850	-172.180	19.805
2000	37.640	146.570	115.997	61.147	-338.356	-163.424	17.858

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 36.376 + 0.722\times10^{-3}T - 7.610\times10^{5}T^{-2}$

$H°- H°_{298} = 36.376\times10^{-3}T + 0.361\times10^{-6}T^{2} + 7.610\times10^{2}T^{-1} - 13.430$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr° = -349.779 + 6.552\times10^{-3}T - 0.457\times10^{-6}T^{2} + 447.400T^{-1}$

$\Delta Gr° = -349.779 - 6.552\times10^{-3}T\ln T + 0.457\times10^{-6}T^{2} + 223.700T^{-1} + 142.114\times10^{-3}T$

Source: Data from Mills (159).

$Te_2F_{10}(g)$
Ditellurium Decafluoride (ideal gas)
[Reaction: $Te_2(g) + 5F_2(g) = Te_2F_{10}(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHr°	ΔGr°	
298.15*	46.970	106.070	106.070	0	-626.330	-567.292	415.831
300	47.130	106.390	106.073	.095	-626.321	-566.929	413.002
400	55.340	121.250	108.052	5.279	-625.861	-547.181	298.962
500	59.170	134.050	112.000	11.025	-625.031	-527.599	230.610
600	61.310	145.050	116.620	17.058	-624.061	-508.204	185.111
700	62.650	154.600	121.371	23.260	-623.028	-488.971	152.662
800	63.560	163.030	126.063	29.574	-621.970	-469.898	128.369
900	64.230	170.560	130.599	35.965	-620.895	-450.952	109.505
1000	64.750	177.360	134.945	42.415	-619.823	-432.138	94.442
1100	65.160	183.550	139.085	48.911	-618.750	-413.413	82.137
1200	65.500	189.230	143.027	55.444	-617.682	-394.788	71.900
1300	65.800	194.490	146.790	62.010	-616.616	-376.259	63.254
1400	66.060	199.370	150.368	68.603	-615.564	-357.810	55.856
1500	66.300	203.940	153.793	75.221	-614.506	-339.443	49.456
1600	66.520	208.220	157.056	81.862	-613.439	-321.135	43.864
1700	66.720	212.260	160.187	88.524	-612.359	-302.883	38.938
1800	66.910	216.080	163.188	95.205	-611.277	-284.721	34.569
1900	67.090	219.700	166.066	101.905	-610.177	-266.600	30.666
2000	67.260	223.150	168.839	108.622	-609.075	-248.555	27.160

*Data estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 65.162 + 1.244\times10^{-3}T - 16.501\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 65.162\times10^{-3}T + 0.622\times10^{-6}T^2 + 16.501\times10^{2}T^{-1} - 25.018$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta Hr^\circ = -634.204 + 14.023\times10^{-3}T - 0.841\times10^{-6}T^2 + 1123.400T^{-1}$

$\Delta Gr^\circ = -634.204 - 14.023\times10^{-3}T\ln T + 0.841\times10^{-6}T^2 + 561.700T^{-1} + 297.753\times10^{-3}T$

Source: Data are estimations from Mills (159).

$ThBr_4(c,l,g)$

Thorium Tetrabromide

[Formation: $Th(c) + 2Br_2(l,g) = ThBr_4(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	29.920	52.820	52.820	.000	-230.783	-221.034	162.020
300*	29.950	53.005	52.822	.055	-230.806	-220.973	160.977
332.6	30.299	56.113	52.995	1.037	-231.214	-219.884	144.483
332.6	30.299	56.113	52.995	1.037	-245.344	-219.884	144.483
400	31.020	61.780	54.005	3.110	-244.900	-214.770	117.343
500	31.710	68.780	56.290	6.245	-244.216	-207.321	90.619
600	32.250	74.610	58.868	9.445	-243.499	-200.005	72.851
693	32.690	79.290	61.301	12.465	-242.815	-193.314	60.964
693	32.690	80.730	61.301	13.465	-241.815	-193.314	60.964
700	32.720	81.060	61.496	13.695	-241.762	-192.824	60.201
800	33.150	85.460	64.223	16.990	-241.003	-185.882	50.780
900	33.560	89.390	66.807	20.325	-240.233	-179.043	43.477
970	33.840	91.910	68.526	22.685	-239.680	-174.303	39.272
970	41.000	107.390	68.526	37.695	-224.670	-174.303	39.272
1000	41.000	108.640	69.715	38.925	-224.218	-172.756	37.755
1100	41.000	112.540	73.426	43.025	-222.726	-167.672	33.313
1127	41.000	113.540	74.382	44.130	-222.329	-166.332	32.255
1127	25.776	136.705	74.382	70.240	-196.219	-166.332	32.255
1200	25.783	138.323	78.222	72.121	-196.260	-164.395	29.940
1300	25.791	140.387	82.926	74.699	-196.334	-161.737	27.190
1400	25.797	142.298	87.099	77.279	-196.427	-159.069	24.832
1500	25.801	144.078	90.839	79.859	-196.543	-156.400	22.787
1600	25.805	145.744	94.220	82.439	-196.679	-153.719	20.997
1633	25.806	146.271	95.266	83.291	-196.729	-152.833	20.454
1633	25.806	146.271	95.266	83.291	-197.589	-152.833	20.454
1700	25.808	147.308	97.296	85.020	-197.649	-150.996	19.412
1800	25.811	148.783	100.116	87.601	-197.766	-148.248	18.000
1900	25.813	150.179	102.715	90.182	-197.913	-145.490	16.735
2000	25.815	151.503	105.122	92.763	-198.093	-142.731	15.597

*Data above 298 K except temperature and enthalpy of fusion and temperature of boiling estimated.

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
693 K, α - β transition point of $ThBr_4$; $\Delta H°$ = 1.000 kcal/mol.
970 K, melting point of $ThBr_4$; $\Delta H°$ = 15.010 kcal/mol.
1127 K, boiling point of $ThBr_4$; $\Delta H°$ = 26.110 kcal/mol.
1633 K, α - β transition point of Th; $\Delta H°$ = 0.860 kcal/mol.

$ThBr_4$(c,l,g) - Continued

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-693 K: $Cp^\circ = 30.340 + 3.838\times10^{-3}T - 1.390\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 30.340\times10^{-3}T + 1.919\times10^{-6}T^2 + 1.390\times10^{2}T^{-1} - 9.683$

693-970 K: $Cp^\circ = 30.503 + 3.610\times10^{-3}T - 1.467\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 30.503\times10^{-3}T + 1.805\times10^{-6}T^2 + 1.467\times10^{2}T^{-1} - 8.752$

970-1127 K: $Cp^\circ = 40.987$

$H^\circ - H^\circ_{298} = 40.987\times10^{-3}T - 2.062$

1127-2000 K: $Cp^\circ = 25.812 + 0.014\times10^{-3}T - 0.669\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.812\times10^{-3}T + 0.007\times10^{-6}T^2 + 0.669\times10^{2}T^{-1} + 41.081$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -227.779 - 11.900\times10^{-3}T + 1.172\times10^{-6}T^2 + 131.100T^{-1}$

$\Delta Gf^\circ = -227.779 + 11.900\times10^{-3}T\ln T - 1.172\times10^{-6}T^2 + 65.550T^{-1} - 45.567\times10^{-3}T$

332.6-693 K: $\Delta Hf^\circ = -247.780 + 6.422\times10^{-3}T + 0.862\times10^{-6}T^2 + 68.300T^{-1}$

$\Delta Gf^\circ = -247.780 - 6.422\times10^{-3}T\ln T - 0.862\times10^{-6}T^2 + 34.150T^{-1} + 121.143\times10^{-3}T$

693-970 K: $\Delta Hf^\circ = -246.849 + 6.585\times10^{-3}T + 0.748\times10^{-6}T^2 + 76.000T^{-1}$

$\Delta Gf^\circ = -246.849 - 6.585\times10^{-3}T\ln T - 0.748\times10^{-6}T^2 + 38.000T^{-1} + 120.779\times10^{-3}T$

970-1127 K: $\Delta Hf^\circ = -240.159 + 17.069\times10^{-3}T - 1.057\times10^{-6}T^2 - 70.700T^{-1}$

$\Delta Gf^\circ = -240.159 - 17.069\times10^{-3}T\ln T + 1.057\times10^{-6}T^2 - 35.350T^{-1} + 184.311\times10^{-3}T$

1127-1633 K: $\Delta Hf^\circ = -197.015 + 1.894\times10^{-3}T - 1.050\times10^{-6}T^2 - 3.800T^{-1}$

$\Delta Gf^\circ = -197.015 - 1.894\times10^{-3}T\ln T + 1.050\times10^{-6}T^2 - 1.900T^{-1} + 39.371\times10^{-3}T$

1633-2000 K: $\Delta Hf^\circ = -200.264 + 4.143\times10^{-3}T - 1.521\times10^{-6}T^2 - 49.400T^{-1}$

$\Delta Gf^\circ = -200.264 - 4.143\times10^{-3}T\ln T + 1.521\times10^{-6}T^2 - 24.700T^{-1} + 57.238\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (256). Entropy at 298 K based on Singh (215). Temperature and enthalpy of fusion and temperature of boiling from Singh (215). Other high-temperature data are those estimated by Wagman (256).

$ThBr_4(g)$

Thorium Tetrabromide (ideal gas)

[Formation: $Th(c) + 2Br_2(l,g) = ThBr_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	25.064	102.720	102.720	0	-181.783	-186.912	137.008
300	25.073	102.875	102.722	.046	-181.815	-186.943	136.186
332.6	25.178	105.467	102.866	.865	-182.386	-187.471	123.185
332.6	25.178	105.467	102.866	.865	-196.516	-187.471	123.185
400	25.396	110.139	103.709	2.572	-196.438	-185.651	101.434
500	25.551	115.824	105.584	5.120	-196.341	-182.968	79.974
600	25.636	120.491	107.691	7.680	-196.264	-180.299	65.673
700	25.688	124.447	109.810	10.246	-196.211	-177.643	55.462
800	25.722	127.879	111.858	12.817	-196.176	-174.990	47.805
900	25.745	130.910	113.810	15.390	-196.168	-172.346	41.851
1000	25.762	133.624	115.658	17.966	-196.177	-169.699	37.087
1100	25.774	136.080	117.405	20.543	-196.208	-167.048	33.189
1200	25.783	138.323	119.055	23.121	-196.260	-164.395	29.940
1300	25.791	140.387	120.619	25.699	-196.334	-161.737	27.190
1400	25.797	142.298	122.099	28.279	-196.427	-159.069	24.832
1500	25.801	144.078	123.505	30.859	-196.543	-156.400	22.787
1600	25.805	145.744	124.845	33.439	-196.679	-153.719	20.997
1633	25.806	146.271	125.272	34.291	-196.729	-152.833	20.454
1633	25.806	146.271	125.272	34.291	-197.589	-152.833	20.454
1700	25.808	147.308	126.120	36.020	-197.649	-150.996	19.412
1800	25.811	148.783	127.338	38.601	-197.766	-148.248	18.000
1900	25.813	150.179	128.504	41.182	-197.913	-145.490	16.735
2000	25.815	151.503	129.622	43.763	-198.093	-142.731	15.597

*Data except enthalpy of formation at 298 estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
1633 K, α - β transition point of Th; ΔH° = 0.860 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 25.812 + 0.014\times10^{-3}T - 0.669\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.812\times10^{-3}T + 0.007\times10^{-6}T^2 + 0.669\times10^{2}T^{-1} - 7.921$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -177.017 - 16.428\times10^{-3}T - 0.740\times10^{-6}T^2 + 59.000T^{-1}$

$\Delta Gf^\circ = -177.017 + 16.428\times10^{-3}T\ln T + 0.740\times10^{-6}T^2 + 29.500T^{-1} - 127.339\times10^{-3}T$

332.6-1633 K: $\Delta Hf^\circ = -197.018 + 1.894\times10^{-3}T - 1.050\times10^{-6}T^2 - 3.800T^{-1}$

$\Delta Gf^\circ = -197.018 - 1.894\times10^{-3}T\ln T + 1.050\times10^{-6}T^2 - 1.900T^{-1} + 39.371\times10^{-3}T$

1633-2000 K: $\Delta Hf^\circ = -200.267 + 4.143\times10^{-3}T - 1.521\times10^{-6}T^2 - 49.400T^{-1}$

$\Delta Gf^\circ = -200.267 - 4.143\times10^{-3}T\ln T + 1.521\times10^{-6}T^2 - 24.700T^{-1} + 57.238\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Singh (215). Other data are those estimated by Wagman (256).

$ThCl_4(c,l)$
Thorium Tetrachloride
[Formation: $Th(c) + 2Cl_2(g) = ThCl_4(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	28.750	45.500	45.500	0	-283.642	-261.627	191.775
300	28.780	45.680	45.503	.053	-283.631	-261.491	190.494
400	30.060	54.150	46.650	3.000	-283.009	-254.204	138.889
500	30.940	60.950	48.846	6.052	-282.350	-247.075	107.995
600	31.680	66.660	51.353	9.184	-281.663	-240.084	87.449
679	32.210	70.610	53.368	11.708	-281.098	-234.646	75.525
679	32.210	72.380	53.368	12.908	-279.898	-234.646	75.525
700	32.340	73.360	53.953	13.585	-279.745	-233.248	72.822
800	32.970	77.720	56.656	16.851	-278.997	-226.657	61.919
900	33.570	81.640	59.219	20.179	-278.216	-220.161	53.462
1000	34.160	85.210	61.645	23.565	-277.403	-213.759	46.716
1042	34.410	86.620	62.623	25.006	-277.050	-211.093	44.274
1042	40.000	100.720	62.623	39.696	-262.360	-211.093	44.274
1100	40.000	102.880	64.684	42.016	-261.550	-208.254	41.376
1200	40.000	106.360	68.013	46.016	-260.174	-203.470	37.057
1300	40.000	109.570	71.096	50.016	-258.820	-198.809	33.422
1400	40.000	112.530	73.947	54.016	-257.489	-194.237	30.321
1500	40.000	115.290	76.613	58.016	-256.181	-189.767	27.649

*Entropy at 298 K estimated.

Phase changes: 679 K, α - β transition point of $ThCl_4$; $\Delta H° = 1.200$ kcal/mol.
1042 K, melting point of $ThCl_4$; $\Delta H° = 14.690$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-679 K:
$$Cp° = 28.756 + 5.560\times10^{-3}T - 1.479\times10^{5}T^{-2}$$
$$H°- H°_{298} = 28.756\times10^{-3}T + 2.780\times10^{-6}T^{2} + 1.479\times10^{2}T^{-1} - 9.317$$

679-1042 K:
$$Cp° = 28.710 + 5.590\times10^{-3}T - 1.368\times10^{5}T^{-2}$$
$$H°- H°_{298} = 28.710\times10^{-3}T + 2.795\times10^{-6}T^{2} + 1.368\times10^{2}T^{-1} - 8.076$$

1042-1500 K:
$$Cp° = 40.000$$
$$H°- H°_{298} = 40.000\times10^{-3}T - 1.984$$

Formation equations (kcal/mol):

298.15-679 K:
$$\Delta Hf° = -285.305 + 5.044\times10^{-3}T + 1.657\times10^{-6}T^{2} + 3.400T^{-1}$$
$$\Delta Gf° = -285.305 - 5.044\times10^{-3}T\ln T - 1.657\times10^{-6}T^{2} + 1.700T^{-1} + 108.630\times10^{-3}T$$

679-1042 K:
$$\Delta Hf° = -284.064 + 4.998\times10^{-3}T + 1.672\times10^{-6}T^{2} - 7.700T^{-1}$$
$$\Delta Gf° = -284.064 - 4.998\times10^{-3}T\ln T - 1.672\times10^{-6}T^{2} - 3.850T^{-1} + 106.525\times10^{-3}T$$

1042-1500 K:
$$\Delta Hf° = -277.972 + 16.288\times10^{-3}T - 1.123\times10^{-6}T^{2} - 144.500T^{-1}$$
$$\Delta Gf° = -277.972 - 16.288\times10^{-3}T\ln T + 1.123\times10^{-6}T^{2} - 72.250T^{-1} + 176.282\times10^{-3}T$$

Source: Data from Wagman (256) who estimated entropy at 298 K.

$ThCl_4(g)$

Thorium Tetrachloride (ideal gas)

[Formation: $Th(c) + 2Cl_2(g) = ThCl_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	24.273	95.000	95.000	0	-230.942	-223.685	163.963
300	24.290	95.150	95.000	.045	-230.939	-223.640	162.920
400	24.922	102.236	95.961	2.510	-230.799	-221.229	120.872
500	25.237	107.835	97.797	5.019	-230.683	-218.850	95.658
600	25.414	112.453	99.866	7.552	-230.595	-216.492	78.856
700	25.523	116.380	101.951	10.100	-230.530	-214.147	66.859
800	25.594	119.793	103.973	12.656	-230.492	-211.810	57.863
900	25.644	122.810	105.901	15.218	-230.477	-209.475	50.867
1000	25.679	125.514	107.730	17.784	-230.484	-207.144	45.271
1100	25.706	127.963	109.460	20.353	-230.513	-204.808	40.691
1200	25.726	130.201	111.097	22.925	-230.565	-202.471	36.874
1300	25.742	132.260	112.646	25.498	-230.638	-200.124	33.644
1400	25.754	134.169	114.117	28.073	-230.732	-197.775	30.874
1500	25.764	135.946	115.513	30.649	-230.848	-195.418	28.472
1600	25.773	137.609	116.843	33.226	-230.985	-193.051	26.369
1633	25.775	138.135	117.268	34.077	-231.035	-192.267	25.731
1633	25.775	138.135	117.268	34.077	-231.895	-192.267	25.731
1700	25.780	139.172	118.111	35.804	-231.956	-190.637	24.508
1800	25.785	140.645	119.322	38.382	-232.076	-188.206	22.851
1900	25.790	142.039	120.481	40.961	-232.225	-185.761	21.367
2000	25.794	143.362	121.592	43.540	-232.409	-183.313	20.031

Phase change: 1633 K, α - β transition point of Th; ΔH° = 0.860 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 25.752 + 0.050\times10^{-3}T - 1.328\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.752\times10^{-3}T + 0.025\times10^{-6}T^2 + 1.328\times10^{2}T^{-1} - 8.126$

Formation equations (kcal/mol):

298.15-1633 K: $\Delta Hf^\circ = -231.413 + 2.040\times10^{-3}T - 1.098\times10^{-6}T^2 - 11.700T^{-1}$

$\Delta Gf^\circ = -231.413 - 2.040\times10^{-3}T\ln T + 1.098\times10^{-6}T^2 - 5.850T^{-1} + 37.283\times10^{-3}T$

1633-2000 K: $\Delta Hf^\circ = -234.662 + 4.289\times10^{-3}T - 1.569\times10^{-6}T^2 - 57.300T^{-1}$

$\Delta Gf^\circ = -234.662 - 4.289\times10^{-3}T\ln T + 1.569\times10^{-6}T^2 - 28.650T^{-1} + 55.150\times10^{-3}T$

Source: Data from Wagman (256).

$ThF_2(g)$

Thorium Difluoride (ideal gas)

[Formation: $Th(c) + F_2(g) = ThF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	12.527	70.533	70.533	0	-156.389	-159.171	116.674
300	12.541	70.611	70.534	.023	-156.392	-159.189	115.967
400	13.064	74.299	71.034	1.306	-156.543	-160.098	87.472
500	13.343	77.247	71.991	2.628	-156.712	-160.968	70.358
600	13.506	79.695	73.077	3.971	-156.906	-161.801	58.935
700	13.609	81.785	74.175	5.327	-157.125	-162.600	50.765
800	13.677	83.607	75.242	6.692	-157.368	-163.365	44.629
900	13.725	85.221	76.263	8.062	-157.636	-164.099	39.848
1000	13.759	86.669	77.233	9.436	-157.927	-164.803	36.017
1100	13.785	87.982	78.151	10.814	-158.239	-165.474	32.876
1200	13.805	89.182	79.021	12.193	-158.575	-166.118	30.254
1300	13.820	90.288	79.846	13.574	-158.931	-166.731	28.030
1400	13.832	91.312	80.628	14.957	-159.309	-167.317	26.119
1500	13.842	92.267	81.373	16.341	-159.708	-167.877	24.459
1600	13.850	93.161	82.083	17.725	-160.128	-168.408	23.003
1633	13.852	93.444	82.310	18.182	-160.272	-168.578	22.561
1633	13.852	93.444	82.310	18.182	-161.132	-168.578	22.561
1700	13.857	94.001	82.759	19.111	-161.381	-168.876	21.710
1800	13.863	94.793	83.406	20.497	-161.783	-169.307	20.556
1900	13.868	95.542	84.025	21.883	-162.214	-169.711	19.521
2000	13.872	96.254	84.619	23.270	-162.677	-170.097	18.587

*Data except enthalpy of formation at 298 K estimated.

Phase change: 1633 K, α - β transition point of Th; ΔH° = 0.860 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.751 + 0.100\times10^{-3}T - 1.114\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.751\times10^{-3}T + 0.050\times10^{-6}T^2 + 1.114\times10^{2}T^{-1} - 4.478$

Formation equations (kcal/mol):

298.15-1633 K: $\Delta Hf^\circ = -156.061 - 0.815\times10^{-3}T - 1.071\times10^{-6}T^2 + 3.000T^{-1}$

$\Delta Gf^\circ = -156.061 + 0.815\times10^{-3}T\ln T + 1.071\times10^{-6}T^2 + 1.500T^{-1} - 15.410\times10^{-3}T$

1633-2000 K: $\Delta Hf^\circ = -159.310 + 1.434\times10^{-3}T - 1.542\times10^{-6}T^2 - 42.600T^{-1}$

$\Delta Gf^\circ = -159.310 - 1.434\times10^{-3}T\ln T + 1.542\times10^{-6}T^2 - 21.300T^{-1} + 2.457\times10^{-3}T$

Source: Data from Wagman (256). All are estimates except enthalpy of formation at 298 K.

$ThF_3(g)$

Thorium Trifluoride (ideal gas)

[Formation: $Th(c) + 1.5F_2(g) = ThF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	17.519	81.072	81.072	0	-283.149	-281.851	206.600
300	17.542	81.181	81.074	.032	-283.150	-281.844	205.321
400	18.431	86.363	81.773	1.836	-283.164	-281.405	153.751
500	18.906	90.532	83.122	3.705	-283.189	-280.963	122.807
600	19.184	94.006	84.654	5.611	-283.234	-280.514	102.176
700	19.358	96.977	86.207	7.539	-283.305	-280.055	87.436
800	19.475	99.570	87.719	9.481	-283.402	-279.585	76.378
900	19.556	101.869	89.167	11.432	-283.525	-279.101	67.774
1000	19.614	103.932	90.541	13.391	-283.671	-278.602	60.888
1100	19.658	105.804	91.845	15.355	-283.840	-278.086	55.250
1200	19.692	107.516	93.081	17.322	-284.034	-277.557	50.549
1300	19.718	109.093	94.252	19.293	-284.247	-277.005	46.568
1400	19.739	110.555	95.365	21.266	-284.485	-276.441	43.154
1500	19.756	111.918	96.424	23.241	-284.744	-275.859	40.192
1600	19.770	113.193	97.432	25.217	-285.025	-275.256	37.598
1633	19.774	113.597	97.755	25.869	-285.123	-275.054	36.811
1633	19.774	113.597	97.755	25.869	-285.983	-275.054	36.811
1700	19.781	114.392	98.396	27.194	-286.141	-274.601	35.302
1800	19.791	115.523	99.316	29.173	-286.406	-273.916	33.258
1900	19.799	116.593	100.197	31.153	-286.700	-273.212	31.426
2000	19.806	117.609	101.043	33.133	-287.029	-272.496	29.777

*Data except enthalpy of formation at 298 K estimated.

Phase change: 1633 K, α - β transition point of Th; $\Delta H° = 0.860$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.598 + 0.172\times10^{-3}T - 1.893\times10^{5}T^{-2}$

$H°- H°_{298} = 19.598\times10^{-3}T + 0.086\times10^{-6}T^{2} + 1.893\times10^{2}T^{-1} - 6.486$

Formation equations (kcal/mol):

298.15-1633 K: $\Delta Hf° = -283.384 + 0.778\times10^{-3}T - 1.122\times10^{-6}T^{2} + 30.650T^{-1}$

$\Delta Gf° = -283.384 - 0.778\times10^{-3}T\ln T + 1.122\times10^{-6}T^{2} + 15.325T^{-1} + 9.067\times10^{-3}T$

1633-2000 K: $\Delta Hf° = -286.633 + 3.027\times10^{-3}T - 1.593\times10^{-6}T^{2} - 14.950T^{-1}$

$\Delta Gf° = -286.633 - 3.027\times10^{-3}T\ln T + 1.593\times10^{-6}T^{2} - 7.475T^{-1} + 26.934\times10^{-3}T$

Source: Data from Wagman (256). All are estimates except enthalpy of formation at 298 K.

ThF_4(c,l)

Thorium Tetrafluoride

[Formation: Th(c) + $2F_2$(g) = ThF_4(c,l)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	26.420	33.950	33.950	0	-501.443	-478.874	351.020
300	26.470	34.110	33.950	.049	-501.434	-478.734	348.753
400	28.130	41.980	35.007	2.789	-500.897	-471.244	257.473
500	29.000	48.360	37.062	5.649	-500.332	-463.897	202.767
600	29.570	53.700	39.402	8.579	-499.769	-456.664	166.338
700	29.990	58.290	41.780	11.557	-499.214	-449.524	140.346
800	30.330	62.320	44.103	14.574	-498.667	-442.465	120.874
900	30.630	65.910	46.330	17.622	-498.128	-435.471	105.745
1000	30.900	69.150	48.451	20.699	-497.596	-428.538	93.656
1100	31.150	72.110	50.472	23.802	-497.069	-421.659	83.775
1200	31.390	74.830	52.389	26.929	-496.548	-414.827	75.549
1300	31.620	77.350	54.212	30.080	-496.029	-408.032	68.596
1383	31.810	79.320	55.667	32.712	-495.604	-402.440	63.595
1383	32.000	86.550	55.667	42.712	-485.604	-402.440	63.595
1400	32.000	86.940	56.043	43.256	-485.514	-401.416	62.663
1500	32.000	89.140	58.169	46.456	-485.000	-395.417	57.611
1600	32.000	91.210	60.175	49.656	-484.510	-389.467	53.198
1633	32.000	91.863	60.809	50.712	-484.354	-387.508	51.861
1633	32.000	91.863	60.809	50.712	-485.214	-387.508	51.861
1700	32.000	93.150	62.058	52.856	-484.857	-383.505	49.302
1800	32.000	94.980	63.838	56.056	-484.357	-377.561	45.842
1900	32.000	96.710	65.523	59.256	-483.887	-371.639	42.748
2000	32.000	98.360	67.132	62.456	-483.454	-365.762	39.968

Phase changes: 1383 K, melting point of ThF_4; ΔH° = 10.000 kcal/mol.
1633 K, α - β transition point of Th; ΔH° = 0.860 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1383 K: $Cp^\circ = 29.200 + 2.000\times10^{-3}T - 3.001\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 29.200\times10^{-3}T + 1.000\times10^{-6}T^2 + 3.001\times10^{2}T^{-1} - 9.801$

1383-2000 K: $Cp^\circ = 32.000$

$H^\circ - H^\circ_{298} = 32.000\times10^{-3}T - 1.544$

Formation equations (kcal/mol):

298.15-1383 K: $\Delta Hf^\circ = -503.549 + 6.126\times10^{-3}T - 0.295\times10^{-6}T^2 + 91.200T^{-1}$

$\Delta Gf^\circ = -503.549 - 6.126\times10^{-3}T\ln T + 0.295\times10^{-6}T^2 + 45.600T^{-1} + 117.063\times10^{-3}T$

1383-1633 K: $\Delta Hf^\circ = -495.292 + 8.926\times10^{-3}T - 1.295\times10^{-6}T^2 - 208.900T^{-1}$

$\Delta Gf^\circ = -495.292 - 8.926\times10^{-3}T\ln T + 1.295\times10^{-6}T^2 - 104.450T^{-1} + 130.037\times10^{-3}T$

1633-2000 K: $\Delta Hf^\circ = -498.540 + 11.175\times10^{-3}T - 1.766\times10^{-6}T^2 - 254.500T^{-1}$

$\Delta Gf^\circ = -498.540 - 11.175\times10^{-3}T\ln T + 1.766\times10^{-6}T^2 - 127.250T^{-1} + 147.904\times10^{-3}T$

Source: Data from Wagman (256).

$ThF_4(g)$

Thorium Tetrafluoride (ideal gas)

[Formation: $Th(c) + 2F_2(g) = ThF_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	22.235	81.667	81.667	0	-422.570	-414.228	303.633
300	22.269	81.805	81.668	.041	-422.569	-414.177	301.724
400	23.598	88.413	82.558	2.342	-422.471	-411.391	224.771
500	24.324	93.765	84.283	4.741	-422.367	-408.635	178.612
600	24.753	98.240	86.245	7.197	-422.278	-405.897	147.846
700	25.025	102.078	88.241	9.686	-422.212	-403.173	125.875
800	25.207	105.432	90.183	12.199	-422.169	-400.456	109.398
900	25.334	108.409	92.047	14.726	-422.151	-397.743	96.584
1000	25.426	111.083	93.819	17.264	-422.158	-395.033	86.333
1100	25.496	113.510	95.500	19.811	-422.187	-392.317	77.945
1200	25.548	115.731	97.095	22.363	-422.241	-389.601	70.955
1300	25.590	117.777	98.608	24.920	-422.316	-386.874	65.039
1400	25.623	119.675	100.046	27.481	-422.416	-384.147	59.967
1500	25.650	121.444	101.415	30.044	-422.539	-381.412	55.571
1600	25.672	123.100	102.719	32.610	-422.683	-378.664	51.722
1633	25.678	123.624	103.136	33.457	-422.736	-377.756	50.556
1633	25.678	123.624	103.136	33.457	-423.596	-377.756	50.556
1700	25.690	124.657	103.964	35.178	-423.662	-375.872	48.321
1800	25.705	126.126	105.155	37.748	-423.792	-373.059	45.295
1900	25.718	127.516	106.295	40.319	-423.951	-370.234	42.586
2000	25.730	128.835	107.389	42.892	-424.145	-367.403	40.147

*Data except enthalpy of formation at 298 K estimated.

Phase change: 1633 K, α - β transition point of Th; $\Delta H° = 0.860$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 25.348 + 0.302\times10^{-3}T - 2.847\times10^{5}T^{-2}$

$H°- H°_{298} = 25.348\times10^{-3}T + 0.151\times10^{-6}T^2 + 2.847\times10^{2}T^{-1} - 8.526$

Formation equations (kcal/mol):

298.15-1633 K: $\Delta Hf° = -423.401 + 2.274\times10^{-3}T - 1.144\times10^{-6}T^2 + 75.800T^{-1}$

$\Delta Gf° = -423.401 - 2.274\times10^{-3}T\ln T + 1.144\times10^{-6}T^2 + 37.900T^{-1} + 42.954\times10^{-3}T$

1633-2000 K: $\Delta Hf° = -426.649 + 4.523\times10^{-3}T - 1.615\times10^{-6}T^2 + 30.200T^{-1}$

$\Delta Gf° = -426.649 - 4.523\times10^{-3}T\ln T + 1.615\times10^{-6}T^2 + 15.100T^{-1} + 60.821\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Nagarajan (170). Other data are estimates from Wagman (256).

$ThI_4(c,l)$
Thorium Tetraiodide
[Formation: $Th(c) + 2I_2(c,l,g) = ThI_4(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	30.270	61.000	61.000	0	-160.566	-158.397	116.106
300	30.300	61.190	61.003	.056	-160.570	-158.384	115.381
386.8	31.185	69.011	61.955	2.729	-160.888	-157.715	89.111
386.8	31.185	69.011	61.955	2.729	-168.306	-157.715	89.111
400	31.320	70.060	62.205	3.142	-168.493	-157.351	85.971
458.4	31.694	74.355	63.483	4.984	-169.300	-155.662	74.214
458.4	31.694	74.355	63.483	4.984	-189.342	-155.662	74.214
500	31.960	77.120	64.504	6.308	-189.050	-152.616	66.707
600	32.450	82.990	67.107	9.530	-188.329	-145.395	52.960
700	32.870	88.030	69.750	12.796	-187.588	-138.302	43.179
800	33.250	92.440	72.313	16.102	-186.830	-131.308	35.871
839	33.390	94.030	73.285	17.402	-186.531	-128.608	33.500
839	42.000	107.730	73.285	28.902	-175.031	-128.608	33.500
900	42.000	110.680	75.720	31.464	-174.043	-125.269	30.419
1000	42.000	115.110	79.446	35.664	-172.438	-119.940	26.213
1100	42.000	119.110	82.870	39.864	-170.856	-114.764	22.801
1200	42.000	122.760	86.040	44.064	-169.298	-109.729	19.984
1300	42.000	126.130	89.004	48.264	-167.758	-104.835	17.624
1400	42.000	129.240	91.766	52.464	-166.243	-100.048	15.618
1500	42.000	132.140	94.364	56.664	-164.749	-95.380	13.897

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
839 K, melting point of ThI_4; ΔH° = 11.500 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-839 K: $Cp^\circ = 31.000 + 3.102\times10^{-3}T - 1.471\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 31.000\times10^{-3}T + 1.551\times10^{-6}T^2 + 1.471\times10^{2}T^{-1} - 9.874$

839-1500 K: $Cp^\circ = 42.000$
$H^\circ - H^\circ_{298} = 42.000\times10^{-3}T - 6.336$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -160.579 - 0.812\times10^{-3}T - 2.380\times10^{-6}T^2 + 139.200T^{-1}$
$\Delta Gf^\circ = -160.579 + 0.812\times10^{-3}T\ln T + 2.380\times10^{-6}T^2 + 69.600T^{-1} + 1.201\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -163.490 - 13.620\times10^{-3}T + 0.604\times10^{-6}T^2 + 139.200T^{-1}$
$\Delta Gf^\circ = -163.490 + 13.620\times10^{-3}T\ln T - 0.604\times10^{-6}T^2 + 69.600T^{-1} - 66.429\times10^{-3}T$

458.4-839 K: $\Delta Hf^\circ = -192.916 + 7.060\times10^{-3}T + 0.468\times10^{-6}T^2 + 108.600T^{-1}$
$\Delta Gf^\circ = -192.916 - 7.060\times10^{-3}T\ln T - 0.468\times10^{-6}T^2 + 54.300T^{-1} + 124.497\times10^{-3}T$

839-1500 K: $\Delta Hf^\circ = -189.378 + 18.060\times10^{-3}T - 1.083\times10^{-6}T^2 - 38.500T^{-1}$
$\Delta Gf^\circ = -189.378 - 18.060\times10^{-3}T\ln T + 1.083\times10^{-6}T^2 - 19.250T^{-1} + 193.137\times10^{-3}T$

Source: Data from Wagman (256). All are estimates except enthalpy of formation at 298 K.

TiBr(g)

Titanium Monobromide (ideal gas)

[Formation: $Ti(c,l) + 0.5Br_2(l,g) = TiBr(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	9.087	62.175	62.175	0	50.800	39.868	-29.224
300	9.098	62.231	62.175	.017	50.789	39.802	-28.995
332.6	9.262	63.178	62.227	.316	50.598	38.618	-25.375
332.6	9.262	63.178	62.227	.316	47.065	38.618	-25.375
400	9.601	64.920	62.537	.953	46.988	36.912	-20.167
500	9.961	67.104	63.240	1.932	46.883	34.403	-15.037
600	10.194	68.943	64.041	2.941	46.785	31.916	-11.625
700	10.333	70.525	64.856	3.968	46.676	29.452	-9.195
800	10.411	71.911	65.655	5.005	46.553	26.998	-7.375
900	10.453	73.140	66.419	6.049	46.409	24.563	-5.965
1000	10.475	74.242	67.147	7.095	46.247	22.146	-4.840
1100	10.489	75.241	67.837	8.144	46.062	19.739	-3.922
1156	10.495	75.762	68.209	8.731	45.948	18.405	-3.480
1156	10.495	75.762	68.209	8.731	44.931	18.405	-3.480
1200	10.500	76.154	68.493	9.193	44.884	17.396	-3.168
1300	10.511	76.995	69.115	10.244	44.762	15.110	-2.540
1400	10.524	77.775	69.707	11.295	44.619	12.833	-2.003
1500	10.539	78.501	70.268	12.349	44.459	10.571	-1.540
1600	10.557	79.182	70.805	13.403	44.277	8.316	-1.136
1700	10.576	79.823	71.317	14.460	44.073	6.074	-.781
1800	10.596	80.428	71.807	15.518	43.839	3.844	-.467
1900	10.618	81.001	72.275	16.579	43.572	1.632	-.188
1945	10.628	81.250	72.480	17.057	43.438	.640	-.072
1945	10.628	81.250	72.480	17.057	40.138	.640	-.072
2000	10.640	81.546	72.725	17.642	39.863	-.474	.052

*Data estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1945 K, melting point of Ti; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 10.442 + 0.116\times10^{-3}T - 1.235\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 10.442\times10^{-3}T + 0.058\times10^{-6}T^2 + 1.235\times10^{2}T^{-1} - 3.533$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = 51.742 - 4.080\times10^{-3}T - 1.015\times10^{-6}T^2 + 108.700T^{-1}$

$\Delta Gf^\circ = 51.742 + 4.080\times10^{-3}T\ln T + 1.015\times10^{-6}T^2 + 54.350T^{-1} - 63.989\times10^{-3}T$

332.6-1156 K: $\Delta Hf^\circ = 46.742 + 0.500\times10^{-3}T - 1.093\times10^{-6}T^2 + 93.000T^{-1}$

$\Delta Gf^\circ = 46.742 - 0.500\times10^{-3}T\ln T + 1.093\times10^{-6}T^2 + 46.500T^{-1} - 22.311\times10^{-3}T$

1156-1945 K: $\Delta Hf^\circ = 42.705 + 2.900\times10^{-3}T - 1.416\times10^{-6}T^2 + 875.900T^{-1}$

$\Delta Gf^\circ = 42.705 - 2.900\times10^{-3}T\ln T + 1.416\times10^{-6}T^2 + 437.950T^{-1} - 2.559\times10^{-3}T$

1945-2000 K: $\Delta Hf^\circ = 49.837 - 5.073\times10^{-3}T + 0.031\times10^{-6}T^2 + 107.800T^{-1}$

$\Delta Gf^\circ = 49.837 + 5.073\times10^{-3}T\ln T - 0.031\times10^{-6}T^2 + 53.900T^{-1} - 63.691\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

$TiBr_2(c,g)$
Titanium Dibromide
[Formation: $Ti(c,l) + Br_2(l,g) = TiBr_2(c,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	18.807	25.900	25.900	0	-96.900	-91.593	67.139
300	18.812	26.016	25.900	.035	-96.909	-91.558	66.699
332.6	18.901	27.961	26.008	.650	-97.079	-90.969	59.774
332.6	18.901	27.961	26.008	.650	-104.144	-90.969	59.774
400	19.086	31.466	26.641	1.930	-103.872	-88.328	48.259
500	19.360	35.754	28.050	3.852	-103.475	-84.490	36.930
600	19.634	39.308	29.638	5.802	-103.077	-80.729	29.405
700	19.908	42.355	31.242	7.779	-102.682	-77.030	24.050
800	20.182	45.032	32.803	9.783	-102.286	-73.395	20.050
900	20.456	47.424	34.296	11.815	-101.891	-69.806	16.951
1000	20.730	49.594	35.720	13.874	-101.490	-66.262	14.481
1100	21.004	51.583	37.073	15.961	-101.088	-62.765	12.470
1156	21.157	52.629	37.801	17.141	-100.861	-60.816	11.498
1156	21.157	52.629	37.801	17.141	-101.878	-60.816	11.498
1200	21.278	53.422	38.360	18.075	-101.652	-59.257	10.792
1208.8	21.302	53.576	38.468	18.262	-101.607	-58.945	10.657
1208.8	14.934	94.352	38.468	67.552	-52.317	-58.945	10.657
1300	14.975	95.437	42.426	68.914	-52.439	-59.439	9.993
1400	15.030	96.549	46.253	70.414	-52.586	-59.972	9.362
1500	15.096	97.588	49.641	71.920	-52.748	-60.494	8.814
1600	15.171	98.565	52.669	73.433	-52.926	-61.006	8.333
1700	15.254	99.487	55.396	74.955	-53.120	-61.504	7.907
1800	15.343	100.362	57.871	76.484	-53.338	-61.994	7.527
1900	15.437	101.194	60.129	78.023	-53.583	-62.466	7.185
1945	15.480	101.556	61.084	78.719	-53.705	-62.675	7.042
1945	15.480	101.556	61.084	78.719	-57.005	-62.675	7.042
2000	15.532	101.988	62.202	79.572	-57.263	-62.833	6.866

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
1156 K, α - β transition point of Ti; $\Delta H°$ = 1.017 kcal/mol.
1208.8 K, sublimation point of $TiBr_2$; $\Delta H°$ = 49.290 kcal/mol.
1945 K, melting point of Ti; $\Delta H°$ = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1208.8 K: $Cp° = 17.991 + 2.738\times10^{-3}T$

$H°- H°_{298} = 17.991\times10^{-3}T + 1.369\times10^{-6}T^2 - 5.486$

1208.8-2000 K: $Cp° = 12.610 + 1.350\times10^{-3}T + 10.105\times10^{5}T^{-2}$

$H°- H°_{298} = 12.610\times10^{-3}T + 0.675\times10^{-6}T^2 - 10.105\times10^{2}T^{-1} + 52.159$

$TiBr_2$(c,g) - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -95.218 - 5.577\times10^{-3}T + 0.346\times10^{-6}T^2 - 14.800T^{-1}$

$\Delta Gf^\circ = -95.218 + 5.577\times10^{-3}T\ln T - 0.346\times10^{-6}T^2 - 7.400T^{-1} - 19.430\times10^{-3}T$

332.6-1156 K: $\Delta Hf^\circ = -105.219 + 3.584\times10^{-3}T + 0.191\times10^{-6}T^2 - 46.200T^{-1}$

$\Delta Gf^\circ = -105.219 - 3.584\times10^{-3}T\ln T - 0.191\times10^{-6}T^2 - 23.100T^{-1} + 63.925\times10^{-3}T$

1156-1208.8 K: $\Delta Hf^\circ = -109.256 + 5.984\times10^{-3}T - 0.132\times10^{-6}T^2 + 736.700T^{-1}$

$\Delta Gf^\circ = -109.256 - 5.984\times10^{-3}T\ln T + 0.132\times10^{-6}T^2 + 368.350T^{-1} + 83.677\times10^{-3}T$

1208.8-1945 K: $\Delta Hf^\circ = -51.611 + 0.603\times10^{-3}T - 0.826\times10^{-6}T^2 - 273.800T^{-1}$

$\Delta Gf^\circ = -51.611 - 0.603\times10^{-3}T\ln T + 0.826\times10^{-6}T^2 - 136.900T^{-1} - 2.694\times10^{-3}T$

1945-2000 K: $\Delta Hf^\circ = -44.479 - 7.370\times10^{-3}T + 0.620\times10^{-6}T^2 - 1041.900T^{-1}$

$\Delta Gf^\circ = -44.479 + 7.370\times10^{-3}T\ln T - 0.620\times10^{-6}T^2 - 520.950T^{-1} - 63.827\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$TiBr_2(g)$

Titanium Dibromide (ideal gas)

[Formation: $Ti(c,l) + Br_2(l,g) = TiBr_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	14.346	73.752	73.752	0	-42.800	-51.760	37.941
300	14.353	73.841	73.752	.027	-42.817	-51.814	37.746
332.6	14.427	75.325	73.834	.496	-43.133	-52.776	34.678
332.6	14.427	75.325	73.834	.496	-50.198	-52.776	34.678
400	14.581	78.005	74.317	1.475	-50.227	-53.298	29.120
500	14.694	81.273	75.395	2.939	-50.288	-54.063	23.630
600	14.756	83.958	76.605	4.412	-50.367	-54.809	19.964
700	14.795	86.235	77.821	5.890	-50.471	-55.535	17.339
800	14.822	88.213	79.000	7.370	-50.599	-56.253	15.367
900	14.844	89.960	80.122	8.854	-50.752	-56.949	13.829
1000	14.867	91.525	81.186	10.339	-50.925	-57.628	12.594
1100	14.894	92.943	82.191	11.827	-51.122	-58.295	11.582
1156	14.914	93.684	82.731	12.661	-51.241	-58.654	11.089
1156	14.914	93.684	82.731	12.661	-52.258	-58.654	11.089
1200	14.930	94.241	83.143	13.318	-52.309	-58.897	10.726
1300	14.975	95.437	84.042	14.814	-52.439	-59.439	9.993
1400	15.030	96.549	84.896	16.314	-52.586	-59.972	9.362
1500	15.096	97.588	85.708	17.820	-52.748	-60.494	8.814
1600	15.171	98.565	86.482	19.333	-52.926	-61.006	8.333
1700	15.254	99.487	87.219	20.855	-53.120	-61.504	7.907
1800	15.343	100.362	87.926	22.384	-53.338	-61.994	7.527
1900	15.437	101.194	88.603	23.923	-53.583	-62.466	7.185
1945	15.480	101.556	88.898	24.619	-53.705	-62.675	7.042
1945	15.480	101.556	88.898	24.619	-57.005	-62.675	7.042
2000	15.532	101.988	89.252	25.472	-57.263	-62.833	6.866

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1945 K, melting point of Ti; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 14.688 + 0.272\times10^{-3}T - 0.376\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.688\times10^{-3}T + 0.136\times10^{-6}T^2 + 0.376\times10^{2}T^{-1} - 4.517$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -40.150 - 8.880\times10^{-3}T - 0.887\times10^{-6}T^2 + 22.800T^{-1}$

$\Delta Gf^\circ = -40.150 + 8.880\times10^{-3}T\ln T + 0.887\times10^{-6}T^2 + 11.400T^{-1} - 89.928\times10^{-3}T$

332.6-1156 K: $\Delta Hf^\circ = -50.150 + 0.281\times10^{-3}T - 1.042\times10^{-6}T^2 - 8.600T^{-1}$

$\Delta Gf^\circ = -50.150 - 0.281\times10^{-3}T\ln T + 1.042\times10^{-6}T^2 - 4.300T^{-1} - 6.573\times10^{-3}T$

1156-1945 K: $\Delta Hf^\circ = -54.187 + 2.681\times10^{-3}T - 1.365\times10^{-6}T^2 + 774.300T^{-1}$

$\Delta Gf^\circ = -54.187 - 2.681\times10^{-3}T\ln T + 1.365\times10^{-6}T^2 + 387.150T^{-1} + 13.179\times10^{-3}T$

1945-2000 K: $\Delta Hf^\circ = -47.055 - 5.292\times10^{-3}T + 0.081\times10^{-6}T^2 + 6.200T^{-1}$

$\Delta Gf^\circ = -47.055 + 5.292\times10^{-3}T\ln T - 0.081\times10^{-6}T^2 + 3.100T^{-1} - 47.953\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$TiBr_3(c)$

Titanium Tribromide

[Formation: $Ti(c) + 1.5Br_2(l,g) = TiBr_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	24.310	42.200	42.200	0	-131.100	-125.230	91.795
300	24.319	42.350	42.200	.045	-131.116	-125.192	91.201
332.6	24.661	44.876	42.341	.843	-131.396	-124.534	81.830
332.6	24.661	44.876	42.341	.843	-141.994	-124.534	81.830
400	25.367	49.467	43.165	2.521	-141.619	-121.035	66.130
500	27.224	55.314	45.024	5.145	-140.961	-115.965	50.687
600	29.734	60.490	47.177	7.988	-140.114	-111.040	40.446
700	32.843	65.299	49.425	11.112	-139.018	-106.271	33.179
800	36.529	69.919	51.700	14.575	-137.611	-101.686	27.779

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
1060 K, calculated sublimation point of $TiBr_3$; $\Delta H°$ = 32 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp° = 9.069 + 32.636\times10^{-3}T + 4.898\times10^{5}T^{-2}$

$H°- H°_{298} = 9.069\times10^{-3}T + 16.318\times10^{-6}T^2 - 4.898\times10^{2}T^{-1} - 2.512$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -123.752 - 23.545\times10^{-3}T + 15.345\times10^{-6}T^2 - 504.600T^{-1}$

$\Delta Gf° = -123.752 + 23.545\times10^{-3}T\ln T - 15.345\times10^{-6}T^2 - 252.300T^{-1} - 131.691\times10^{-3}T$

332.6-800 K: $\Delta Hf° = -138.752 - 9.803\times10^{-3}T + 15.113\times10^{-6}T^2 - 551.700T^{-1}$

$\Delta Gf° = -138.752 + 9.803\times10^{-3}T\ln T - 15.113\times10^{-6}T^2 - 275.850T^{-1} - 6.659\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (254). Low-temperature heat capacities and entropy at 298 K from King (129). High-temperature data based on King.

$TiBr_3(g)$
Titanium Tribromide (ideal gas)
[Formation: $Ti(c,l) + 1.5Br_2(l,g) = TiBr_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	18.961	85.777	85.777	0	-89.600	-96.722	70.898
300	18.985	85.895	85.778	.035	-89.625	-96.765	70.492
332.6	19.271	87.868	85.888	.659	-90.081	-97.518	64.078
332.6	19.271	87.868	85.888	.659	-100.678	-97.518	64.078
400	19.862	91.493	86.535	1.983	-100.656	-96.883	52.934
500	20.271	95.974	87.990	3.992	-100.614	-95.948	41.938
600	20.462	99.689	89.639	6.030	-100.572	-95.017	34.610
700	20.547	102.851	91.307	8.081	-100.549	-94.089	29.375
800	20.579	105.597	92.924	10.138	-100.548	-93.166	25.451
900	20.587	108.021	94.470	12.196	-100.576	-92.242	22.399
1000	20.585	110.191	95.936	14.255	-100.625	-91.313	19.956
1100	20.579	112.152	97.322	16.313	-100.703	-90.384	17.957
1156	20.575	113.173	98.065	17.466	-100.756	-89.852	16.987
1156	20.575	113.173	98.065	17.466	-101.773	-89.852	16.987
1200	20.571	113.942	98.633	18.371	-101.774	-89.399	16.282
1300	20.562	115.589	99.876	20.427	-101.797	-88.369	14.856
1400	20.553	117.112	101.053	22.483	-101.841	-87.333	13.633
1500	20.544	118.530	102.171	24.538	-101.908	-86.295	12.573
1600	20.535	119.855	103.235	26.592	-102.000	-85.250	11.644
1700	20.526	121.100	104.250	28.645	-102.118	-84.201	10.825
1800	20.518	122.273	105.219	30.697	-102.268	-83.144	10.095
1900	20.509	123.382	106.146	32.748	-102.457	-82.073	9.440
1945	20.505	123.862	106.551	33.671	-102.558	-81.590	9.168
1945	20.505	123.862	106.551	33.671	-105.858	-81.590	9.168
2000	20.501	124.434	107.035	34.799	-106.092	-80.903	8.841

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.
1156 K, α - β transition point of Ti; $\Delta H° = 1.017$ kcal/mol.
1945 K, melting point of Ti; $\Delta H° = 3.300$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 21.204 - 0.392\times10^{-3}T - 1.889\times10^{5}T^{-2}$

$H°- H°_{298} = 21.204\times10^{-3}T - 0.196\times10^{-6}T^2 + 1.889\times10^{2}T^{-1} - 6.938$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -86.678 - 11.410\times10^{-3}T - 1.169\times10^{-6}T^2 + 174.100T^{-1}$

$\Delta Gf° = -86.678 + 11.410\times10^{-3}T\ln T + 1.169\times10^{-6}T^2 + 87.050T^{-1} - 100.023\times10^{-3}T$

332.6-1156 K: $\Delta Hf° = -101.679 + 2.332\times10^{-3}T - 1.402\times10^{-6}T^2 + 127.000T^{-1}$

$\Delta Gf° = -101.679 - 2.332\times10^{-3}T\ln T + 1.402\times10^{-6}T^2 + 63.500T^{-1} + 25.010\times10^{-3}T$

1156-1945 K: $\Delta Hf° = -105.716 + 4.732\times10^{-3}T - 1.724\times10^{-6}T^2 + 909.900T^{-1}$

$\Delta Gf° = -105.716 - 4.732\times10^{-3}T\ln T + 1.724\times10^{-6}T^2 + 454.950T^{-1} + 44.763\times10^{-3}T$

1945-2000 K: $\Delta Hf° = -98.584 - 3.241\times10^{-3}T - 0.278\times10^{-6}T^2 + 141.800T^{-1}$

$\Delta Gf° = -98.584 + 3.241\times10^{-3}T\ln T + 0.278\times10^{-6}T^2 + 70.900T^{-1} - 16.370\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$TiBr_4$(c,l,g)
Titanium Tetrabromide
[Formation: $Ti(c,l) + 2Br_2(l,g) = TiBr_4(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	31.431	58.200	58.200	0	-147.400	-140.877	103.264
300	31.499	58.395	58.202	.058	-147.419	-140.835	102.597
311.4	31.936	59.578	58.228	.420	-147.537	-140.582	98.663
311.4	36.110	69.596	58.228	3.540	-144.417	-140.582	98.663
332.6	36.110	71.974	59.029	4.306	-144.544	-140.317	92.201
332.6	36.110	71.974	59.029	4.306	-158.674	-140.317	92.201
400	36.110	78.637	61.790	6.739	-157.838	-136.683	74.679
500	36.110	86.695	65.995	10.350	-156.634	-131.537	57.494
504	36.110	86.982	66.158	10.495	-156.586	-131.336	56.951
504	25.156	108.208	66.158	21.193	-145.888	-131.336	56.951
600	25.350	112.613	73.250	23.618	-145.806	-128.571	46.831
700	25.475	116.531	79.161	26.159	-145.740	-125.700	39.245
800	25.557	119.938	84.049	28.711	-145.691	-122.840	33.558
900	25.614	122.952	88.208	31.270	-145.668	-119.986	29.136
1000	25.655	125.653	91.820	33.833	-145.663	-117.132	25.599
1100	25.686	128.099	95.007	36.401	-145.682	-114.282	22.706
1156	25.699	129.375	96.642	37.839	-145.703	-112.680	21.303
1156	25.699	129.375	96.642	37.839	-146.720	-112.680	21.303
1200	25.709	130.335	97.860	38.970	-146.694	-111.385	20.286
1300	25.727	132.394	100.439	41.542	-146.653	-108.446	18.231
1400	25.742	134.301	102.790	44.116	-146.632	-105.506	16.470
1500	25.753	136.078	104.951	46.690	-146.634	-102.570	14.944
1600	25.763	137.740	106.949	49.266	-146.658	-99.631	13.609
1700	25.771	139.302	108.806	51.843	-146.707	-96.691	12.430
1800	25.778	140.775	110.541	54.421	-146.787	-93.746	11.382
1900	25.783	142.169	112.170	56.999	-146.905	-90.792	10.443
1945	25.785	142.773	112.871	58.159	-146.974	-89.463	10.052
1945	25.785	142.773	112.871	58.159	-150.274	-89.463	10.052
2000	25.788	143.492	113.704	59.577	-150.470	-87.746	9.588

Phase changes: 311.4 K, melting point of $TiBr_4$; ΔH° = 3.120 kcal/mol.
332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
504 K, boiling point of $TiBr_4$; ΔH° = 10.698 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1945 K, melting point of Ti; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-311.4 K: $Cp^\circ = 20.134 + 37.892\times10^{-3}T$

$H^\circ - H^\circ_{298} = 20.134\times10^{-3}T + 18.946\times10^{-6}T^2 - 7.687$

311.4-504 K: $Cp^\circ = 36.111$

$H^\circ - H^\circ_{298} = 36.111\times10^{-3}T - 7.705$

504-2000 K: $Cp^\circ = 25.785 + 0.030\times10^{-3}T - 1.636\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.785\times10^{-3}T + 0.015\times10^{-6}T^2 + 1.636\times10^{2}T^{-1} + 7.869$

$TiBr_4$(c,l,g) - Continued

Formation equations (kcal/mol):

298.15-311.4 K: $\Delta Hf^\circ = -142.535 - 21.525\times10^{-3}T + 18.023\times10^{-6}T^2 - 14.800T^{-1}$

$\Delta Gf^\circ = -142.535 + 21.525\times10^{-3}T\ln T - 18.023\times10^{-6}T^2 - 7.400T^{-1} - 111.624\times10^{-3}T$

311.4-332.6 K: $\Delta Hf^\circ = -142.553 - 5.548\times10^{-3}T - 0.923\times10^{-6}T^2 - 14.800T^{-1}$

$\Delta Gf^\circ = -142.553 + 5.548\times10^{-3}T\ln T + 0.923\times10^{-6}T^2 - 7.400T^{-1} - 25.741\times10^{-3}T$

332.6-504 K: $\Delta Hf^\circ = -162.554 + 12.774\times10^{-3}T - 1.233\times10^{-6}T^2 - 77.600T^{-1}$

$\Delta Gf^\circ = -162.554 - 12.774\times10^{-3}T\ln T + 1.233\times10^{-6}T^2 - 38.800T^{-1} + 140.970\times10^{-3}T$

504-1156 K: $\Delta Hf^\circ = -146.980 + 2.448\times10^{-3}T - 1.218\times10^{-6}T^2 + 86.000T^{-1}$

$\Delta Gf^\circ = -146.980 - 2.448\times10^{-3}T\ln T + 1.218\times10^{-6}T^2 + 43.000T^{-1} + 45.500\times10^{-3}T$

1156-1945 K: $\Delta Hf^\circ = -151.017 + 4.848\times10^{-3}T - 1.541\times10^{-6}T^2 + 868.900T^{-1}$

$\Delta Gf^\circ = -151.017 - 4.848\times10^{-3}T\ln T + 1.541\times10^{-6}T^2 + 434.450T^{-1} + 65.253\times10^{-3}T$

1945-2000 K: $\Delta Hf^\circ = -143.885 - 3.125\times10^{-3}T - 0.095\times10^{-6}T^2 + 100.800T^{-1}$

$\Delta Gf^\circ = -143.885 + 3.125\times10^{-3}T\ln T + 0.095\times10^{-6}T^2 + 50.400T^{-1} + 4.120\times10^{-3}T$

Sources: Enthalpy of formation at 298 K for crystal and gas from Wagman (254). Low-temperature heat capacities and entropy at 298 K from King (129). High-temperature data for crystal and liquid based on King (129). Gas data from JANAF (60).

$TiBr_4(g)$

Titanium Tetrabromide (ideal gas)

[Formation: $Ti(c,l) + 2Br_2(l,g) = TiBr_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	24.070	95.246	95.246	0	-131.300	-135.822	99.559
300	24.089	95.395	95.246	.045	-131.332	-135.848	98.964
332.6	24.319	97.892	95.384	.834	-131.916	-136.309	89.567
332.6	24.319	97.892	95.384	.834	-146.046	-136.309	89.567
400	24.793	102.434	96.201	2.493	-145.984	-134.348	73.403
500	25.148	108.008	98.024	4.992	-145.892	-131.452	57.457
600	25.350	112.613	100.083	7.518	-145.806	-128.571	46.831
700	25.475	116.531	102.161	10.059	-145.740	-125.700	39.245
800	25.557	119.938	104.174	12.611	-145.691	-122.840	33.558
900	25.614	122.952	106.096	15.170	-145.668	-119.986	29.136
1000	25.655	125.653	107.920	17.733	-145.663	-117.132	25.599
1100	25.686	128.099	109.644	20.301	-145.682	-114.283	22.706
1156	25.699	129.375	110.569	21.739	-145.703	-112.680	21.303
1156	25.699	129.375	110.569	21.739	-146.720	-112.680	21.303
1200	25.709	130.335	111.277	22.870	-146.694	-111.385	20.286
1300	25.727	132.394	112.823	25.442	-146.653	-108.446	18.231
1400	25.742	134.301	114.290	28.016	-146.632	-105.506	16.470
1500	25.753	136.078	115.685	30.590	-146.634	-102.570	14.944
1600	25.763	137.740	117.011	33.166	-146.658	-99.631	13.609
1700	25.771	139.302	118.277	35.743	-146.707	-96.691	12.430
1800	25.778	140.775	119.486	38.321	-146.787	-93.746	11.382
1900	25.783	142.169	120.643	40.899	-146.905	-90.792	10.443
1945	25.785	142.773	121.148	42.059	-146.974	-89.463	10.052
1945	25.785	142.773	121.148	42.059	-150.274	-89.463	10.052
2000	25.788	143.492	121.754	43.477	-150.470	-87.746	9.588

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.
1156 K, α - β transition point of Ti; $\Delta H° = 1.017$ kcal/mol.
1945 K, melting point of Ti; $\Delta H° = 3.300$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 25.714 + 0.072\times10^{-3}T - 1.480\times10^{5}T^{-2}$

$H°- H°_{298} = 25.714\times10^{-3}T + 0.036\times10^{-6}T^2 + 1.480\times10^{2}T^{-1} - 8.166$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -126.914 - 15.945\times10^{-3}T - 0.887\times10^{-6}T^2 + 133.200T^{-1}$

$\Delta Gf° = -126.914 + 15.945\times10^{-3}T\ln T + 0.887\times10^{-6}T^2 + 66.600T^{-1} - 121.741\times10^{-3}T$

332.6-1156 K: $\Delta Hf° = -146.915 + 2.377\times10^{-3}T - 1.197\times10^{-6}T^2 + 70.400T^{-1}$

$\Delta Gf° = -146.915 - 2.377\times10^{-3}T\ln T + 1.197\times10^{-6}T^2 + 35.200T^{-1} + 44.969\times10^{-3}T$

1156-1945 K: $\Delta Hf° = -150.952 + 4.777\times10^{-3}T - 1.520\times10^{-6}T^2 + 853.300T^{-1}$

$\Delta Gf° = -150.952 - 4.777\times10^{-3}T\ln T + 1.520\times10^{-6}T^2 + 426.650T^{-1} + 64.722\times10^{-3}T$

1945-2000 K: $\Delta Hf° = -143.820 - 3.196\times10^{-3}T - 0.074\times10^{-6}T^2 + 85.200T^{-1}$

$\Delta Gf° = -143.820 + 3.196\times10^{-3}T\ln T + 0.074\times10^{-6}T^2 + 42.600T^{-1} + 3.589\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (254). Other data from JANAF (60).

TiCl(g)

Titanium Monochloride (ideal gas)

[Formation: $Ti(c,l) + 0.5Cl_2(g) = TiCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	8.915	59.538	59.538	0	36.900	29.275	-21.459
300	8.927	59.593	59.538	.017	36.898	29.230	-21.293
400	9.491	62.243	59.896	.939	36.790	26.689	-14.582
500	9.883	64.406	60.588	1.909	36.690	24.174	-10.566
600	10.135	66.232	61.380	2.911	36.594	21.680	-7.897
700	10.285	67.806	62.189	3.932	36.486	19.208	-5.997
800	10.370	69.186	62.978	4.966	36.365	16.747	-4.575
900	10.416	70.410	63.738	6.005	36.221	14.304	-3.473
1000	10.442	71.509	64.461	7.048	36.059	11.878	-2.596
1100	10.458	72.505	65.148	8.093	35.872	9.463	-1.880
1156	10.465	73.025	65.517	8.679	35.759	8.124	-1.536
1156	10.465	73.025	65.517	8.679	34.742	8.124	-1.536
1200	10.470	73.416	65.799	9.140	34.694	7.112	-1.295
1300	10.481	74.254	66.418	10.187	34.569	4.819	-.810
1400	10.494	75.031	67.005	11.236	34.425	2.536	-.396
1500	10.509	75.756	67.565	12.286	34.262	.264	-.038
1600	10.526	76.434	68.098	13.338	34.078	-1.996	.273
1700	10.545	77.073	68.608	14.391	33.871	-4.244	.546
1800	10.564	77.676	69.094	15.447	33.635	-6.481	.787
1900	10.585	78.248	69.562	16.504	33.364	-8.701	1.001
1945	10.594	78.496	69.766	16.981	33.228	-9.697	1.090
1945	10.594	78.496	69.766	16.981	29.928	-9.697	1.090
2000	10.606	78.792	70.010	17.564	29.652	-10.814	1.182

*Data estimated.

Phase changes: 1156 K, α - β transition point of Ti; $\Delta H°$ = 1.017 kcal/mol.
1945 K, melting point of Ti; $\Delta H°$ = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 10.418 + 0.114\times10^{-3}T - 1.366\times10^{5}T^{-2}$

$H°- H°_{298} = 10.418\times10^{-3}T + 0.057\times10^{-6}T^{2} + 1.366\times10^{2}T^{-1} - 3.569$

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf° = 36.547 + 0.528\times10^{-3}T - 1.110\times10^{-6}T^{2} + 87.650T^{-1}$

$\Delta Gf° = 36.547 - 0.528\times10^{-3}T\ln T + 1.110\times10^{-6}T^{2} + 43.825T^{-1} - 22.209\times10^{-3}T$

1156-1945 K: $\Delta Hf° = 32.510 + 2.928\times10^{-3}T - 1.433\times10^{-6}T^{2} + 870.550T^{-1}$

$\Delta Gf° = 32.510 - 2.928\times10^{-3}T\ln T + 1.433\times10^{-6}T^{2} + 435.275T^{-1} - 2.456\times10^{-3}T$

1945-2000 K: $\Delta Hf° = 39.643 - 5.045\times10^{-3}T + 0.013\times10^{-6}T^{2} + 102.450T^{-1}$

$\Delta Gf° = 39.643 + 5.045\times10^{-3}T\ln T - 0.013\times10^{-6}T^{2} + 51.225T^{-1} - 63.589\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

$TiCl_2(c,g)$
Titanium Dichloride
[Formation: $Ti(c,l) + Cl_2(g) = TiCl_2(c,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	16.690	20.876	20.876	0	-123.200	-111.353	81.623
300*	16.706	20.979	20.876	.031	-123.195	-111.279	81.065
400	17.541	25.902	21.542	1.744	-122.928	-107.347	58.651
500	18.280	29.897	22.825	3.536	-122.632	-103.486	45.233
600	18.732	33.270	24.292	5.387	-122.314	-99.686	36.310
700	19.184	36.192	25.789	7.282	-121.986	-95.936	29.952
800	19.636	38.783	27.254	9.223	-121.644	-92.240	25.198
900	20.088	41.122	28.666	11.210	-121.285	-88.583	21.511
1000	20.540	43.262	30.021	13.241	-120.906	-84.970	18.570
1100	20.992	45.240	31.315	15.318	-120.509	-81.401	16.173
1156	21.245	46.289	32.015	16.500	-120.279	-79.413	15.013
1156	21.245	46.289	32.015	16.500	-121.296	-79.413	15.013
1200	21.444	47.086	32.553	17.439	-121.063	-77.823	14.173
1300	21.896	48.821	33.739	19.606	-120.519	-74.243	12.481
1400	22.348	50.460	34.875	21.819	-119.951	-70.703	11.037
1500	22.800	52.017	35.966	24.076	-119.360	-67.205	9.792
1581.5	23.168	53.233	36.825	25.950	-118.862	-64.385	8.897
1581.5	15.132	90.818	36.825	85.390	-59.422	-64.385	8.897
1600	15.146	90.994	37.450	85.670	-59.456	-64.443	8.802
1700	15.232	91.915	40.627	87.189	-59.652	-64.747	8.324
1800	15.324	92.788	43.501	88.716	-59.872	-65.043	7.897
1900	15.419	93.619	46.117	90.254	-60.118	-65.320	7.513
1945	15.463	93.980	47.220	90.949	-60.241	-65.443	7.353
1945	15.463	93.980	47.220	90.949	-63.541	-65.443	7.353
2000	15.516	94.412	48.512	91.800	-63.802	-65.494	7.157

*Data above 298 K estimated.

Phase changes: 1156 K, α - β transition point of Ti; $\Delta H°$ = 1.017 kcal/mol.
1581.5 K, sublimation point of $TiCl_2$; $\Delta H°$ = 59.440 kcal/mol.
1945 K, melting point of Ti; $\Delta H°$ = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1581.5 K: $Cp° = 16.356 + 4.302\times10^{-3}T - 0.842\times10^{5}T^{-2}$

$H°- H°_{298} = 16.356\times10^{-3}T + 2.151\times10^{-6}T^{2} + 0.842\times10^{2}T^{-1} - 5.350$

1581.5-2000 K: $Cp° = 13.035 + 1.154\times10^{-3}T + 6.787\times10^{5}T^{-2}$

$H°- H°_{298} = 13.035\times10^{-3}T + 0.577\times10^{-6}T^{2} - 6.787\times10^{2}T^{-1} + 63.761$

$TiCl_2(c,g)$ - Continued

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf^\circ = -123.899 + 2.052\times10^{-3}T + 0.940\times10^{-6}T^2 + 1.100T^{-1}$

$\Delta Gf^\circ = -123.899 - 2.052\times10^{-3}T\ln T - 0.940\times10^{-6}T^2 + 0.550T^{-1} + 54.044\times10^{-3}T$

1156-1581.5 K: $\Delta Hf^\circ = -127.936 + 4.452\times10^{-3}T + 0.617\times10^{-6}T^2 + 784.000T^{-1}$

$\Delta Gf^\circ = -127.936 - 4.452\times10^{-3}T\ln T - 0.617\times10^{-6}T^2 + 392.000T^{-1} + 73.797\times10^{-3}T$

1581.5-1945 K: $\Delta Hf^\circ = -58.825 + 1.131\times10^{-3}T - 0.957\times10^{-6}T^2 + 21.100T^{-1}$

$\Delta Gf^\circ = -58.825 - 1.131\times10^{-3}T\ln T + 0.957\times10^{-6}T^2 + 10.550T^{-1} + 3.297\times10^{-3}T$

1945-2000 K: $\Delta Hf^\circ = -51.693 - 6.842\times10^{-3}T + 0.489\times10^{-6}T^2 - 747.000T^{-1}$

$\Delta Gf^\circ = -51.693 + 6.842\times10^{-3}T\ln T - 0.489\times10^{-6}T^2 - 373.500T^{-1} - 57.836\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except values at 298 K.

$TiCl_2(g)$

Titanium Dichloride (ideal gas)

[Formation: $Ti(c,l) + Cl_2(g) = TiCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	13.743	66.500	66.500	0	-56.700	-58.456	42.849
300	13.756	66.585	66.502	.025	-56.701	-58.466	42.592
400	14.218	70.614	67.047	1.427	-56.745	-59.049	32.262
500	14.452	73.814	68.090	2.862	-56.806	-59.618	26.059
600	14.585	76.462	69.272	4.314	-56.887	-60.174	21.918
700	14.668	78.717	70.464	5.777	-56.991	-60.709	18.954
800	14.724	80.679	71.620	7.247	-57.120	-61.233	16.728
900	14.766	82.416	72.726	8.721	-57.274	-61.737	14.992
1000	14.803	83.974	73.774	10.200	-57.447	-62.223	13.599
1100	14.842	85.386	74.766	11.682	-57.645	-62.697	12.457
1156	14.866	86.124	75.300	12.513	-57.765	-62.950	11.901
1156	14.866	86.124	75.300	12.513	-58.782	-62.950	11.901
1200	14.885	86.680	75.707	13.168	-58.834	-63.107	11.493
1300	14.937	87.873	76.597	14.659	-58.966	-63.458	10.668
1500	15.068	90.019	78.246	17.659	-59.277	-64.125	9.343
1600	15.146	90.994	79.013	19.170	-59.456	-64.443	8.802
1700	15.232	91.915	79.745	20.689	-59.652	-64.747	8.324
1800	15.324	92.788	80.446	22.216	-59.872	-65.043	7.897
1900	15.419	93.619	81.117	23.754	-60.118	-65.320	7.513
1945	15.463	93.980	81.410	24.449	-60.241	-65.443	7.353
1945	15.463	93.980	81.410	24.449	-63.541	-65.443	7.353
2000	15.516	94.412	81.762	25.300	-63.802	-65.494	7.157

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1156 K, α - β transition point of Ti; $\Delta H°$ = 1.017 kcal/mol.
1945 K, melting point of Ti; $\Delta H°$ = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 14.627 + 0.312\times10^{-3}T - 0.869\times10^{5}T^{-2}$

$H°- H°_{298} = 14.627\times10^{-3}T + 0.156\times10^{-6}T^{2} + 0.869\times10^{2}T^{-1} - 4.666$

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf° = -56.715 + 0.323\times10^{-3}T - 1.055\times10^{-6}T^{2} + 3.800T^{-1}$

$\Delta Gf° = -56.715 - 0.323\times10^{-3}T\ln T + 1.055\times10^{-6}T^{2} + 1.900T^{-1} - 4.334\times10^{-3}T$

1156-1945 K: $\Delta Hf° = -60.752 + 2.723\times10^{-3}T - 1.378\times10^{-6}T^{2} + 786.700T^{-1}$

$\Delta Gf° = -60.752 - 2.723\times10^{-3}T\ln T + 1.378\times10^{-6}T^{2} + 393.350T^{-1} + 15.418\times10^{-3}T$

1945-2000 K: $\Delta Hf° = -53.620 - 5.250\times10^{-3}T + 0.068\times10^{-6}T^{2} + 18.600T^{-1}$

$\Delta Gf° = -53.620 + 5.250\times10^{-3}T\ln T - 0.068\times10^{-6}T^{2} + 9.300T^{-1} - 45.715\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$TiCl_3(c)$
Titanium Trichloride
[Formation: $Ti(c) + 1.5Cl_2(g) = TiCl_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	23.220	33.400	33.400	0	-172.300	-156.243	114.528
300	23.230	33.544	33.401	.043	-172.290	-156.143	113.748
400	23.676	40.289	34.317	2.389	-171.806	-150.834	82.411
500	24.077	45.616	36.062	4.777	-171.340	-145.646	63.661
600	24.431	50.037	38.034	7.202	-170.883	-140.551	51.195
700	24.739	53.827	40.026	9.661	-170.430	-135.526	42.313
800	25.000	57.148	41.962	12.149	-169.984	-130.572	35.670
900	25.216	60.106	43.817	14.660	-169.546	-125.671	30.517
1000	25.385	62.772	45.582	17.190	-169.115	-120.819	26.405

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 22.999 + 2.548\times10^{-3}T - 0.479\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 22.999\times10^{-3}T + 1.274\times10^{-6}T^2 + 0.479\times10^{2}T^{-1} - 7.131$

Formation equations (kcal/mol):

298.15-1000 K: $\Delta Hf^\circ = -173.346 + 4.282\times10^{-3}T + 0.019\times10^{-6}T^2 - 69.350T^{-1}$

$\Delta Gf^\circ = -173.346 - 4.282\times10^{-3}T\ln T - 0.019\times10^{-6}T^2 - 34.675T^{-1} + 82.152\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (254). Low-temperature heat capacities and entropy at 298 K from King (129). High-temperature data based on King.

$TiCl_3(g)$

Titanium Trichloride (ideal gas)

[Formation: $Ti(c,l) + 1.5Cl_2(g) = TiCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	17.344	75.703	75.703	0	-129.500	-126.056	92.400
300	17.380	75.811	75.704	.032	-129.501	-126.034	91.814
400	18.796	81.027	76.405	1.849	-129.546	-124.869	68.225
500	19.531	85.309	77.771	3.769	-129.548	-123.701	54.069
600	19.924	88.908	79.335	5.744	-129.540	-122.532	44.632
700	20.139	91.997	80.928	7.748	-129.542	-121.358	37.889
800	20.261	94.695	82.484	9.769	-129.564	-120.190	32.834
900	20.333	97.086	83.976	11.799	-129.607	-119.014	28.900
1000	20.377	99.231	85.397	13.834	-129.671	-117.835	25.752
1100	20.406	101.175	86.745	15.873	-129.760	-116.654	23.177
1156	20.416	102.188	87.468	17.017	-129.820	-115.981	21.927
1156	20.416	102.188	87.468	17.017	-130.837	-115.981	21.927
1200	20.424	102.951	88.022	17.915	-130.843	-115.416	21.020
1300	20.437	104.586	89.234	19.958	-130.874	-114.129	19.187
1400	20.445	106.101	90.385	22.002	-130.927	-112.839	17.615
1500	20.450	107.512	91.481	24.047	-131.001	-111.544	16.252
1600	20.452	108.832	92.524	26.092	-131.100	-110.245	15.059
1700	20.453	110.072	93.521	28.137	-131.225	-108.935	14.004
1800	20.452	111.241	94.473	30.183	-131.381	-107.622	13.067
1900	20.450	112.346	95.384	32.228	-131.576	-106.292	12.226
1945	20.449	112.825	95.782	33.148	-131.679	-105.692	11.876
1945	20.449	112.825	95.782	33.148	-134.979	-105.692	11.876
2000	20.448	113.395	96.258	34.273	-135.219	-104.863	11.459

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1945 K, melting point of Ti; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 20.858 - 0.180\times10^{-3}T - 3.077\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 20.858\times10^{-3}T - 0.090\times10^{-6}T^2 + 3.077\times10^{2}T^{-1} - 7.243$

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf^\circ = -130.657 + 2.140\times10^{-3}T - 1.345\times10^{-6}T^2 + 190.450T^{-1}$

$\Delta Gf^\circ = -130.657 - 2.140\times10^{-3}T\ln T + 1.345\times10^{-6}T^2 + 95.225T^{-1} + 26.157\times10^{-3}T$

1156-1945 K: $\Delta Hf^\circ = -134.694 + 4.540\times10^{-3}T - 1.668\times10^{-6}T^2 + 973.350T^{-1}$

$\Delta Gf^\circ = -134.694 - 4.540\times10^{-3}T\ln T + 1.668\times10^{-6}T^2 + 486.675T^{-1} + 45.910\times10^{-3}T$

1945-2000 K: $\Delta Hf^\circ = -127.562 - 3.433\times10^{-3}T - 0.222\times10^{-6}T^2 + 205.250T^{-1}$

$\Delta Gf^\circ = -127.562 + 3.433\times10^{-3}T\ln T + 0.222\times10^{-6}T^2 + 102.625T^{-1} - 15.223\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (254). Other data are those estimated by JANAF (60).

$TiCl_4(l,g)$
Titanium Tetrachloride
[Formation: $Ti(c,l) + 2Cl_2(g) = TiCl_4(l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	34.704	60.326	60.326	0	-192.200	-176.227	129.176
300	34.709	60.541	60.328	.064	-192.177	-176.127	128.307
400	34.936	70.557	61.689	3.547	-190.970	-170.961	93.407
409	34.956	71.330	61.888	3.862	-190.864	-170.509	91.111
409	24.062	92.225	61.888	12.408	-182.318	-170.509	91.111
500	24.610	97.118	67.864	14.627	-182.239	-167.889	73.383
600	24.962	101.639	73.127	17.107	-182.161	-165.027	60.110
700	25.183	105.504	77.483	19.615	-182.098	-162.170	50.631
800	25.330	108.877	81.201	22.141	-182.057	-159.330	43.526
900	25.433	111.867	84.446	24.679	-182.037	-156.489	38.000
1000	25.507	114.551	87.324	27.227	-182.035	-153.650	33.580
1100	25.563	116.985	89.912	29.780	-182.059	-150.818	29.964
1156	25.587	118.255	91.254	31.213	-182.082	-149.223	28.211
1156	25.587	118.255	91.254	31.213	-183.099	-149.223	28.211
1200	25.605	119.211	92.262	32.339	-183.075	-147.934	26.942
1300	25.639	121.262	94.415	34.901	-183.038	-145.008	24.378
1400	25.665	123.163	96.402	37.466	-183.022	-142.083	22.180
1500	25.686	124.934	98.245	40.034	-183.026	-139.157	20.275
1600	25.704	126.592	99.965	42.603	-183.055	-136.233	18.608
1700	25.719	128.151	101.577	45.175	-183.107	-133.300	17.137
1800	25.731	129.622	103.096	47.747	-183.193	-130.374	15.829
1900	25.741	131.013	104.528	50.321	-183.315	-127.430	14.658
1945	25.745	131.616	105.148	51.479	-183.386	-126.107	14.170
1945	25.745	131.616	105.148	51.479	-186.686	-126.107	14.170
2000	25.750	132.334	105.886	52.895	-186.886	-124.394	13.593

Phase changes: 409 K, boiling point of $TiCl_4$; $\Delta H° = 8.546$ kcal/mol.
1156 K, α - β transition point of Ti; $\Delta H° = 1.017$ kcal/mol.
1945 K, melting point of Ti; $\Delta H° = 3.300$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-409 K: $Cp° = 33.973 + 2.452\times10^{-3}T$
$H°-H°_{298} = 33.973\times10^{-3}T + 1.226\times10^{-6}T^2 - 10.238$
409-2000 K: $Cp° = 25.701 + 0.076\times10^{-3}T - 2.794\times10^{5}T^{-2}$
$H°-H°_{298} = 25.701\times10^{-3}T + 0.038\times10^{-6}T^2 + 2.794\times10^{2}T^{-1} + 1.207$

Formation equations (kcal/mol):

298.15-409 K: $\Delta Hf° = -194.918 + 10.842\times10^{-3}T - 0.073\times10^{-6}T^2 - 151.400T^{-1}$
$\Delta Gf° = -194.918 - 10.842\times10^{-3}T\ln T + 0.073\times10^{-6}T^2 - 75.700T^{-1} + 125.294\times10^{-3}T$
409-1156 K: $\Delta Hf° = -183.473 + 2.570\times10^{-3}T - 1.261\times10^{-6}T^2 + 128.000T^{-1}$
$\Delta Gf° = -183.473 - 2.570\times10^{-3}T\ln T + 1.261\times10^{-6}T^2 + 64.000T^{-1} + 46.245\times10^{-3}T$
1156-1945 K: $\Delta Hf° = -187.510 + 4.970\times10^{-3}T - 1.584\times10^{-6}T^2 + 910.900T^{-1}$
$\Delta Gf° = -187.510 - 4.970\times10^{-3}T\ln T + 1.584\times10^{-6}T^2 + 455.450T^{-1} + 65.998\times10^{-3}T$
1945-2000 K: $\Delta Hf° = -180.378 - 3.003\times10^{-3}T - 0.138\times10^{-6}T^2 + 142.800T^{-1}$
$\Delta Gf° = -180.378 + 3.003\times10^{-3}T\ln T + 0.138\times10^{-6}T^2 + 71.400T^{-1} + 4.865\times10^{-3}T$

Source: Data from JANAF (60).

$TiCl_4(g)$

Titanium Tetrachloride (ideal gas)

[Formation: $Ti(c,l) + 2Cl_2(g) = TiCl_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	22.852	84.793	84.793	0	-182.400	-173.722	127.340
300	22.881	84.935	84.795	.042	-182.399	-173.667	126.515
400	24.008	91.690	85.708	2.393	-182.324	-170.768	93.302
500	24.610	97.118	87.464	4.827	-182.239	-167.889	73.383
600	24.962	101.639	89.461	7.307	-182.161	-165.027	60.110
700	25.183	105.504	91.483	9.815	-182.098	-162.170	50.631
800	25.330	108.877	93.451	12.341	-182.057	-159.330	43.526
900	25.433	111.867	95.335	14.879	-182.037	-156.489	38.000
1000	25.507	114.551	97.124	17.427	-182.035	-153.650	33.580
1100	25.563	116.985	98.821	19.980	-182.059	-150.818	29.964
1156	25.587	118.255	99.732	21.413	-182.082	-149.223	28.211
1156	25.587	118.255	99.732	21.413	-183.099	-149.223	28.211
1200	25.605	119.211	100.428	22.539	-183.075	-147.934	26.942
1300	25.639	121.262	101.954	25.101	-183.038	-145.008	24.378
1400	25.665	123.163	103.402	27.666	-183.022	-142.083	22.180
1500	25.686	124.934	104.778	30.234	-183.026	-139.157	20.275
1600	25.704	126.592	106.090	32.803	-183.055	-136.233	18.608
1700	25.719	128.151	107.342	35.375	-183.107	-133.300	17.137
1800	25.731	129.622	108.540	37.947	-183.193	-130.374	15.829
1900	25.741	131.013	109.686	40.521	-183.315	-127.430	14.658
1945	25.745	131.616	110.187	41.679	-183.386	-126.107	14.170
1945	25.745	131.616	110.187	41.679	-186.686	-126.107	14.170
2000	25.750	132.334	110.786	43.095	-186.886	-124.394	13.593

Phase changes: 1156 K, α - β transition point of Ti; $\Delta H° = 1.017$ kcal/mol.
1945 K, melting point of Ti; $\Delta H° = 3.300$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 25.527 + 0.180\times10^{-3}T - 2.425\times10^{5}T^{-2}$

$H°- H°_{298} = 25.527\times10^{-3}T + 0.090\times10^{-6}T^2 + 2.425\times10^{2}T^{-1} - 8.432$

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf° = -183.312 + 2.396\times10^{-3}T - 1.209\times10^{-6}T^2 + 91.100T^{-1}$

$\Delta Gf° = -183.312 - 2.396\times10^{-3}T\ln T + 1.209\times10^{-6}T^2 + 45.550T^{-1} + 44.946\times10^{-3}T$

1156-1945 K: $\Delta Hf° = -187.349 + 4.796\times10^{-3}T - 1.532\times10^{-6}T^2 + 874.000T^{-1}$

$\Delta Gf° = -187.349 - 4.796\times10^{-3}T\ln T + 1.532\times10^{-6}T^2 + 437.000T^{-1} + 64.698\times10^{-3}T$

1945-2000 K: $\Delta Hf° = -180.217 - 3.177\times10^{-3}T - 0.086\times10^{-6}T^2 + 105.900T^{-1}$

$\Delta Gf° = -180.217 + 3.177\times10^{-3}T\ln T + 0.086\times10^{-6}T^2 + 52.950T^{-1} + 3.566\times10^{-3}T$

Source: Data from JANAF (60).

TiF(g)

Titanium Monofluoride (ideal gas)

[Formation: $Ti(c,l) + 0.5F_2(g) = TiF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	8.446	56.692	56.692	0	-16.000	-23.499	17.225
300	8.461	56.744	56.692	.016	-16.002	-23.544	17.151
400	9.156	59.279	57.034	.898	-16.121	-26.040	14.227
500	9.636	61.377	57.697	1.840	-16.223	-28.509	12.461
600	9.942	63.163	58.463	2.820	-16.323	-30.957	11.276
700	10.128	64.711	59.248	3.824	-16.432	-33.382	10.422
800	10.236	66.071	60.017	4.843	-16.557	-35.797	9.779
900	10.298	67.281	60.759	5.870	-16.703	-38.192	9.274
1000	10.334	68.368	61.466	6.902	-16.869	-40.569	8.866
1100	10.357	69.354	62.139	7.936	-17.061	-42.937	8.531
1156	10.366	69.869	62.501	8.517	-17.177	-44.248	8.365
1156	10.366	69.869	62.501	8.517	-18.194	-44.248	8.365
1200	10.373	70.256	62.778	8.973	-18.245	-45.239	8.239
1300	10.387	71.087	63.386	10.011	-18.375	-47.483	7.983
1400	10.401	71.857	63.964	11.050	-18.527	-49.718	7.761
1500	10.417	72.575	64.514	12.091	-18.698	-51.938	7.567
1600	10.433	73.248	65.039	13.134	-18.890	-54.149	7.396
1700	10.450	73.881	65.541	14.178	-19.106	-56.345	7.244
1800	10.469	74.479	66.021	15.224	-19.352	-58.530	7.106
1900	10.487	75.045	66.481	16.271	-19.633	-60.698	6.982
1945	10.496	75.291	66.682	16.743	-19.774	-61.669	6.929
1945	10.496	75.291	66.682	16.743	-23.074	-61.669	6.929
2000	10.506	75.584	66.924	17.321	-23.357	-62.758	6.858

*Data estimated.

Phase changes: 1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1945 K, melting point of Ti; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 10.282 + 0.160\times10^{-3}T - 1.674\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 10.282\times10^{-3}T + 0.080\times10^{-6}T^2 + 1.674\times10^{2}T^{-1} - 3.634$

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf^\circ = -16.407 + 0.551\times10^{-3}T - 1.130\times10^{-6}T^2 + 102.350T^{-1}$

$\Delta Gf^\circ = -16.407 - 0.551\times10^{-3}T\ln T + 1.130\times10^{-6}T^2 + 51.175T^{-1} - 21.558\times10^{-3}T$

1156-1945 K: $\Delta Hf^\circ = -20.444 + 2.951\times10^{-3}T - 1.453\times10^{-6}T^2 + 885.250T^{-1}$

$\Delta Gf^\circ = -20.444 - 2.951\times10^{-3}T\ln T + 1.453\times10^{-6}T^2 + 442.625T^{-1} - 1.806\times10^{-3}T$

1945-2000 K: $\Delta Hf^\circ = -13.312 - 5.022\times10^{-3}T - 0.007\times10^{-6}T^2 + 117.150T^{-1}$

$\Delta Gf^\circ = -13.312 + 5.022\times10^{-3}T\ln T + 0.007\times10^{-6}T^2 + 58.575T^{-1} - 62.938\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

$TiF_2(g)$

Titanium Difluoride (ideal gas)

[Formation: $Ti(c,l) + F_2(g) = TiF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	12.638	61.081	61.081	0	-164.500	-166.086	121.742
300	12.659	61.159	61.082	.023	-164.502	-166.095	120.999
400	13.486	64.927	61.590	1.335	-164.575	-166.614	91.032
500	13.942	67.990	62.574	2.708	-164.649	-167.118	73.046
600	14.213	70.557	63.695	4.117	-164.734	-167.603	61.049
700	14.387	72.762	64.836	5.548	-164.840	-168.067	52.472
800	14.504	74.692	65.951	6.993	-164.970	-168.522	46.037
900	14.590	76.405	67.018	8.448	-165.124	-168.954	41.027
1000	14.660	77.946	68.036	9.910	-165.300	-169.371	37.016
1100	14.722	79.346	69.001	11.379	-165.500	-169.775	33.731
1156	14.757	80.078	69.520	12.205	-165.620	-169.986	32.137
1156	14.757	80.078	69.520	12.205	-166.637	-169.986	32.137
1200	14.784	80.630	69.917	12.855	-166.690	-170.112	30.981
1300	14.850	81.816	70.788	14.336	-166.825	-170.392	28.645
1400	14.923	82.919	71.615	15.825	-166.977	-170.662	26.641
1500	15.002	83.951	72.404	17.321	-167.144	-170.918	24.902
1600	15.089	84.922	73.156	18.826	-167.327	-171.164	23.380
1700	15.181	85.840	73.876	20.339	-167.528	-171.397	22.034
1800	15.278	86.710	74.564	21.862	-167.753	-171.619	20.837
1900	15.378	87.539	75.226	23.395	-168.005	-171.826	19.764
1945	15.423	87.900	75.515	24.088	-168.131	-171.916	19.317
1945	15.423	87.900	75.515	24.088	-171.431	-171.916	19.317
2000	15.479	88.330	75.862	24.937	-171.695	-171.927	18.787

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1156 K, α - β transition point of Ti; $\Delta H°$ = 1.017 kcal/mol.
1945 K, melting point of Ti; $\Delta H°$ = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 14.384 + 0.462\times10^{-3}T - 1.674\times10^{5}T^{-2}$

$H°- H°_{298} = 14.384\times10^{-3}T + 0.231\times10^{-6}T^2 + 1.674\times10^{2}T^{-1} - 4.871$

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf° = -164.699 + 0.399\times10^{-3}T - 1.066\times10^{-6}T^2 + 52.100T^{-1}$

$\Delta Gf° = -164.699 - 0.399\times10^{-3}T\ln T + 1.066\times10^{-6}T^2 + 26.050T^{-1} - 2.988\times10^{-3}T$

1156-1945 K: $\Delta Hf° = -168.736 + 2.799\times10^{-3}T - 1.389\times10^{-6}T^2 + 835.000T^{-1}$

$\Delta Gf° = -168.736 - 2.799\times10^{-3}T\ln T + 1.389\times10^{-6}T^2 + 417.500T^{-1} + 16.764\times10^{-3}T$

1945-2000 K: $\Delta Hf° = -161.604 - 5.174\times10^{-3}T + 0.057\times10^{-6}T^2 + 66.900T^{-1}$

$\Delta Gf° = -161.604 + 5.174\times10^{-3}T\ln T - 0.057\times10^{-6}T^2 + 33.450T^{-1} - 44.368\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$TiF_3(c,g)$
Titanium Trifluoride
[Formation: $Ti(c,l) + 1.5F_2(g) = TiF_3(c,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	21.994	21.000	21.000	0	-343.100	-325.514	238.605
300	22.000	21.136	21.000	.041	-343.091	-325.404	237.053
400	22.300	27.497	21.865	2.253	-342.649	-319.575	174.606
500	22.970	32.545	23.513	4.516	-342.235	-313.857	137.185
600	23.536	36.783	25.381	6.841	-341.819	-308.222	112.268
700	24.128	40.455	27.278	9.224	-341.397	-302.649	94.490
800	24.746	43.717	29.132	11.668	-340.958	-297.146	81.175
900	25.390	46.669	30.920	14.174	-340.497	-291.695	70.832
1000	26.060	49.378	32.631	16.747	-340.002	-286.297	62.569
1100	26.756	51.894	34.269	19.387	-339.474	-280.958	55.821
1156	27.160	53.232	35.156	20.897	-339.160	-277.984	52.554
1156	27.160	53.232	35.156	20.897	-340.177	-277.984	52.554
1200	27.478	54.253	35.837	22.099	-339.874	-275.623	50.197
1300	28.226	56.482	37.340	24.884	-339.152	-270.296	45.440
1308.3	28.290	56.662	37.461	25.120	-339.089	-269.855	45.078
1308.3	20.254	97.478	37.461	78.520	-285.689	-269.855	45.078
1400	20.284	98.851	41.438	80.378	-285.749	-268.746	41.953
1500	20.309	100.252	45.313	82.408	-285.834	-267.528	38.978
1600	20.328	101.563	48.789	84.439	-285.944	-266.305	36.375
1700	20.342	102.796	51.930	86.473	-286.078	-265.071	34.077
1800	20.353	103.959	54.788	88.508	-286.247	-263.833	32.033
1900	20.361	105.059	57.405	90.543	-286.453	-262.579	30.203
1945	20.364	105.536	58.513	91.459	-286.562	-262.014	29.441
1945	20.364	105.536	58.513	91.459	-289.862	-262.014	29.441
2000	20.367	106.104	59.814	92.580	-290.107	-261.224	28.545

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1308.3 K, sublimation point of TiF_3; ΔH° = 53.400 kcal/mol.
1945 K, melting point of Ti; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1308.3 K: $Cp^\circ = 19.214 + 6.828\times10^{-3}T + 0.660\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.214\times10^{-3}T + 3.414\times10^{-6}T^2 - 0.660\times10^{2}T^{-1} - 5.811$

1308.3-2000 K: $Cp^\circ = 20.539 - 0.034\times10^{-3}T - 4.136\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 20.539\times10^{-3}T - 0.017\times10^{-6}T^2 + 4.136\times10^{2}T^{-1} + 51.362$

TiF_3(c,g) - Continued

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf^\circ = -342.795 + 0.975\times10^{-3}T + 2.030\times10^{-6}T^2 - 231.550T^{-1}$

$\Delta Gf^\circ = -342.795 - 0.975\times10^{-3}T\ln T - 2.030\times10^{-6}T^2 - 115.775T^{-1} + 65.423\times10^{-3}T$

1156-1308.3 K: $\Delta Hf^\circ = -346.832 + 3.375\times10^{-3}T + 1.707\times10^{-6}T^2 + 551.350T^{-1}$

$\Delta Gf^\circ = -346.832 - 3.375\times10^{-3}T\ln T - 1.707\times10^{-6}T^2 + 275.675T^{-1} + 85.175\times10^{-3}T$

1308.3-1945 K: $\Delta Hf^\circ = -289.659 + 4.700\times10^{-3}T - 1.724\times10^{-6}T^2 + 1030.950T^{-1}$

$\Delta Gf^\circ = -289.659 - 4.700\times10^{-3}T\ln T + 1.724\times10^{-6}T^2 + 515.475T^{-1} + 46.355\times10^{-3}T$

1945-2000 K: $\Delta Hf^\circ = -282.527 - 3.273\times10^{-3}T - 0.278\times10^{-6}T^2 + 262.850T^{-1}$

$\Delta Gf^\circ = -282.527 + 3.273\times10^{-3}T\ln T + 0.278\times10^{-6}T^2 + 131.425T^{-1} - 14.777\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$TiF_3(g)$
Titanium Trifluoride (ideal gas)
[Formation: $Ti(c,l) + 1.5F_2(g) = TiF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	15.675	69.622	69.622	0	-284.100	-281.010	205.984
300	15.718	69.719	69.622	.029	-284.103	-280.991	204.699
400	17.513	74.509	70.262	1.699	-284.203	-279.934	152.947
500	18.567	78.541	71.527	3.507	-284.244	-278.864	121.890
600	19.190	81.986	72.989	5.398	-284.262	-277.787	101.182
700	19.569	84.975	74.494	7.337	-284.284	-276.700	86.389
800	19.808	87.605	75.971	9.307	-284.319	-275.617	75.294
900	19.965	89.947	77.396	11.296	-284.375	-274.523	66.662
1000	20.074	92.057	78.759	13.298	-284.451	-273.425	59.756
1100	20.151	93.974	80.056	15.310	-284.551	-272.323	54.105
1156	20.183	94.976	80.755	16.439	-284.617	-271.696	51.365
1156	20.183	94.976	80.755	16.439	-285.634	-271.696	51.365
1200	20.209	95.730	81.290	17.328	-285.645	-271.166	49.385
1300	20.251	97.349	82.464	19.351	-285.685	-269.956	45.383
1400	20.284	98.851	83.581	21.378	-285.749	-268.746	41.953
1500	20.309	100.252	84.647	23.408	-285.834	-267.528	38.978
1600	20.328	101.563	85.664	25.439	-285.944	-266.305	36.375
1700	20.342	102.796	86.635	27.473	-286.078	-265.071	34.077
1800	20.353	103.959	87.566	29.508	-286.247	-263.833	32.033
1900	20.361	105.059	88.457	31.543	-286.453	-262.579	30.203
1945	20.364	105.536	88.847	32.459	-286.562	-262.014	29.441
1945	20.364	105.536	88.847	32.459	-289.862	-262.014	29.441
2000	20.367	106.104	89.314	33.580	-290.107	-261.224	28.545

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1156 K, α - β transition point of Ti; $\Delta H° = 1.017$ kcal/mol.
1945 K, melting point of Ti; $\Delta H° = 3.300$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 20.077 + 0.300\times10^{-3}T - 3.993\times10^{5}T^{-2}$

$H°- H°_{298} = 20.077\times10^{-3}T + 0.150\times10^{-6}T^2 + 3.993\times10^{2}T^{-1} - 7.339$

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf° = -285.322 + 1.838\times10^{-3}T - 1.234\times10^{-6}T^2 + 233.750T^{-1}$

$\Delta Gf° = -285.322 - 1.838\times10^{-3}T\ln T + 1.234\times10^{-6}T^2 + 116.875T^{-1} + 23.252\times10^{-3}T$

1156-1945 K: $\Delta Hf° = -289.359 + 4.238\times10^{-3}T - 1.557\times10^{-6}T^2 + 1016.650T^{-1}$

$\Delta Gf° = -289.359 - 4.238\times10^{-3}T\ln T + 1.557\times10^{-6}T^2 + 508.325T^{-1} + 43.004\times10^{-3}T$

1945-2000 K: $\Delta Hf° = -282.227 - 3.735\times10^{-3}T - 0.111\times10^{-6}T^2 + 248.550T^{-1}$

$\Delta Gf° = -282.227 + 3.735\times10^{-3}T\ln T + 0.111\times10^{-6}T^2 + 124.275T^{-1} - 18.129\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

TiF_4(c,g)

Titanium Tetrafluoride

[Formation: $Ti(c,l) + 2F_2(g) = TiF_4(c,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	27.310	32.016	32.016	0	-394.190	-372.667	273.168
300	27.390	32.185	32.016	.051	-394.178	-372.532	271.386
400*	30.270	40.483	33.128	2.942	-393.441	-365.422	199.655
500	32.160	47.451	35.315	6.068	-392.566	-358.519	156.706
556.8	32.910	50.958	36.734	7.920	-392.026	-354.681	139.214
556.8	23.605	89.078	36.734	29.145	-370.801	-354.681	139.214
600	23.905	90.853	40.570	30.170	-370.788	-353.432	128.736
700	24.364	94.575	48.025	32.585	-370.758	-350.536	109.441
800	24.682	97.850	54.052	35.038	-370.742	-347.651	94.973
900	24.908	100.771	59.084	37.518	-370.742	-344.762	83.719
1000	25.075	103.405	63.387	40.018	-370.760	-341.875	74.716
1100	25.201	105.801	67.136	42.532	-370.801	-338.990	67.350
1156	25.255	107.054	69.039	43.945	-370.833	-337.367	63.781
1156	25.255	107.054	69.039	43.945	-371.850	-337.367	63.781
1200	25.298	107.998	70.451	45.057	-371.833	-336.055	61.203
1300	25.375	110.026	73.418	47.591	-371.810	-333.073	55.994
1400	25.436	111.909	76.101	50.131	-371.811	-330.097	51.530
1500	25.486	113.665	78.546	52.678	-371.830	-327.113	47.660
1600	25.527	115.312	80.794	55.228	-371.874	-324.133	44.274
1700	25.562	116.860	82.870	57.783	-371.941	-321.143	41.285
1800	25.591	118.322	84.800	60.340	-372.044	-318.156	38.629
1900	25.615	119.706	86.600	62.901	-372.181	-315.154	36.251
1945	25.624	120.306	87.373	64.054	-372.259	-313.804	35.260
1945	25.624	120.306	87.373	64.054	-375.559	-313.804	35.260
2000	25.636	121.021	88.290	65.463	-375.768	-312.058	34.100

*Data above 300 K estimated.

Phase changes: 556.8 K, sublimation point of TiF_4; ΔH° = 21.225 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1945 K, melting point of Ti; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-556.8 K: $Cp^\circ = 28.146 + 10.910\times10^{-3}T - 3.635\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 28.146\times10^{-3}T + 5.455\times10^{-6}T^2 + 3.635\times10^{2}T^{-1} - 10.096$

556.8-2000 K: $Cp^\circ = 25.546 + 0.144\times10^{-3}T - 6.268\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.546\times10^{-3}T + 0.072\times10^{-6}T^2 + 6.268\times10^{2}T^{-1} + 13.773$

TiF_4(c,g) - Continued

Formation equations (kcal/mol):

298.15-556.8 K: $\Delta Hf^\circ = -396.725 + 5.653\times10^{-3}T + 3.984\times10^{-6}T^2 + 147.700T^{-1}$

$\Delta Gf^\circ = -396.725 - 5.653\times10^{-3}T\ln T - 3.984\times10^{-6}T^2 + 73.850T^{-1} + 113.258\times10^{-3}T$

556.8-1156 K: $\Delta Hf^\circ = -372.856 + 3.053\times10^{-3}T - 1.399\times10^{-6}T^2 + 411.000T^{-1}$

$\Delta Gf^\circ = -372.856 - 3.053\times10^{-3}T\ln T + 1.399\times10^{-6}T^2 + 205.500T^{-1} + 50.531\times10^{-3}T$

1156-1945 K: $\Delta Hf^\circ = -376.893 + 5.453\times10^{-3}T - 1.722\times10^{-6}T^2 + 1193.900T^{-1}$

$\Delta Gf^\circ = -376.893 - 5.453\times10^{-3}T\ln T + 1.722\times10^{-6}T^2 + 596.950T^{-1} + 70.283\times10^{-3}T$

1945-2000 K: $\Delta Hf^\circ = -369.761 - 2.520\times10^{-3}T - 0.276\times10^{-6}T^2 + 425.800T^{-1}$

$\Delta Gf^\circ = -369.761 + 2.520\times10^{-3}T\ln T + 0.276\times10^{-6}T^2 + 212.900T^{-1} + 9.151\times10^{-3}T$

Source: Data from JANAF (60) who estimated all above 300 K.

$TiF_4(g)$

Titanium Tetrafluoride (ideal gas)

[Formation: $Ti(c,l) + 2F_2(g) = TiF_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	20.357	75.243	75.243	0	-370.820	-362.185	265.485
300	20.397	75.369	75.243	.038	-370.821	-362.130	263.808
400	22.126	81.492	76.067	2.170	-370.843	-359.228	196.270
500	23.211	86.556	77.672	4.442	-370.822	-356.327	155.748
600	23.905	90.853	79.520	6.800	-370.788	-353.432	128.736
700	24.364	94.575	81.411	9.215	-370.758	-350.536	109.441
800	24.682	97.850	83.265	11.668	-370.742	-347.651	94.973
900	24.908	100.771	85.051	14.148	-370.742	-344.762	83.719
1000	25.075	103.405	86.757	16.648	-370.760	-341.875	74.716
1100	25.201	105.801	88.381	19.162	-370.801	-338.990	67.350
1156	25.255	107.054	89.255	20.575	-370.833	-337.367	63.781
1156	25.255	107.054	89.255	20.575	-371.850	-337.367	63.781
1200	25.298	107.998	89.925	21.687	-371.833	-336.055	61.203
1300	25.375	110.026	91.394	24.221	-371.810	-333.073	55.994
1400	25.436	111.909	92.794	26.761	-371.811	-330.097	51.530
1500	25.486	113.665	94.126	29.308	-371.830	-327.113	47.660
1600	25.527	115.312	95.401	31.858	-371.874	-324.133	44.274
1700	25.562	116.860	96.617	34.413	-371.941	-321.143	41.285
1800	25.591	118.322	97.783	36.970	-372.044	-318.156	38.629
1900	25.615	119.706	98.900	39.531	-372.181	-315.154	36.251
1945	25.624	120.306	99.389	40.684	-372.259	-313.804	35.260
1945	25.624	120.306	99.389	40.684	-375.559	-313.804	35.260
2000	25.636	121.021	99.975	42.093	-375.768	-312.058	34.100

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1156 K, α - β transition point of Ti; $\Delta H°$ = 1.017 kcal/mol.
1945 K, melting point of Ti; $\Delta H°$ = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 24.414 + 0.874\times10^{-3}T - 3.838\times10^{5}T^{-2}$

$H°- H°_{298} = 24.414\times10^{-3}T + 0.437\times10^{-6}T^2 + 3.838\times10^{2}T^{-1} - 8.605$

Formation equations (kcal/mol):

298.15-1156 K: $\Delta Hf° = -371.864 + 1.921\times10^{-3}T - 1.034\times10^{-6}T^2 + 168.000T^{-1}$

$\Delta Gf° = -371.864 - 1.921\times10^{-3}T\ln T + 1.034\times10^{-6}T^2 + 84.000T^{-1} + 42.157\times10^{-3}T$

1156-1945 K: $\Delta Hf° = -375.901 + 4.321\times10^{-3}T - 1.357\times10^{-6}T^2 + 950.900T^{-1}$

$\Delta Gf° = -375.901 - 4.321\times10^{-3}T\ln T + 1.357\times10^{-6}T^2 + 475.450T^{-1} + 61.910\times10^{-3}T$

1945-2000 K: $\Delta Hf° = -368.769 - 3.652\times10^{-3}T + 0.089\times10^{-6}T^2 + 182.800T^{-1}$

$\Delta Gf° = -368.769 + 3.652\times10^{-3}T\ln T - 0.089\times10^{-6}T^2 + 91.400T^{-1} + 0.777\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

TiI(g)

Titanium Monoiodide (ideal gas)

[Formation: $Ti(c,l) + 0.5I_2(c,l,g) = TiI(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	9.192	64.225	64.225	0	65.500	52.672	-38.609
300	9.201	64.281	64.225	.017	65.494	52.594	-38.314
386.8	9.609	66.673	64.514	.835	65.175	48.902	-27.630
386.8	9.609	66.673	64.514	.835	63.320	48.902	-27.630
400	9.671	66.996	64.591	.962	63.237	48.411	-26.450
458.4	9.872	68.329	64.984	1.533	62.873	46.271	-22.060
458.4	9.872	68.329	64.984	1.533	57.862	46.271	-22.060
500	10.015	69.193	65.299	1.947	57.820	45.222	-19.766
600	10.239	71.040	66.105	2.961	57.722	42.712	-15.557
700	10.374	72.630	66.927	3.992	57.614	40.224	-12.558
800	10.451	74.021	67.730	5.033	57.491	37.745	-10.311
900	10.493	75.254	68.497	6.081	57.350	35.287	-8.569
1000	10.517	76.361	69.230	7.131	57.189	32.845	-7.178
1100	10.532	77.364	69.924	8.184	57.005	30.414	-6.043
1156	10.539	77.887	70.297	8.774	56.893	29.066	-5.495
1156	10.539	77.887	70.297	8.774	55.876	29.066	-5.495
1200	10.545	78.281	70.583	9.238	55.830	28.046	-5.108
1300	10.558	79.126	71.208	10.293	55.709	25.735	-4.326
1400	10.573	79.909	71.803	11.349	55.569	23.434	-3.658
1500	10.591	80.639	72.367	12.408	55.411	21.146	-3.081
1600	10.611	81.323	72.906	13.468	55.232	18.867	-2.577
1700	10.632	81.967	73.420	14.530	55.030	16.601	-2.134
1800	10.656	82.575	73.912	15.594	54.800	14.345	-1.742
1900	10.680	83.152	74.383	16.661	54.535	12.106	-1.393
1945	10.691	83.402	74.589	17.142	54.402	11.101	-1.247
1945	10.691	83.402	74.589	17.142	51.102	11.101	-1.247
2000	10.705	83.700	74.835	17.730	50.829	9.975	-1.090

*Data estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1945 K, melting point of Ti; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 10.449 + 0.142\times10^{-3}T - 1.155\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 10.449\times10^{-3}T + 0.071\times10^{-6}T^2 + 1.155\times10^{2}T^{-1} - 3.509$

TiI(g) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = 65.759 - 1.466\times10^{-3}T - 1.798\times10^{-6}T^2 + 100.700T^{-1}$

$\Delta Gf^\circ = 65.759 + 1.466\times10^{-3}T\ln T + 1.798\times10^{-6}T^2 + 50.350T^{-1} - 53.354\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = 65.032 - 4.668\times10^{-3}T - 1.052\times10^{-6}T^2 + 100.700T^{-1}$

$\Delta Gf^\circ = 65.032 + 4.668\times10^{-3}T\ln T + 1.052\times10^{-6}T^2 + 50.350T^{-1} - 70.261\times10^{-3}T$

458.4-1156 K: $\Delta Hf^\circ = 57.675 + 0.502\times10^{-3}T - 1.086\times10^{-6}T^2 + 93.050T^{-1}$

$\Delta Gf^\circ = 57.675 - 0.502\times10^{-3}T\ln T + 1.086\times10^{-6}T^2 + 46.525T^{-1} - 22.530\times10^{-3}T$

1156-1945 K: $\Delta Hf^\circ = 53.638 + 2.902\times10^{-3}T - 1.409\times10^{-6}T^2 + 875.950T^{-1}$

$\Delta Gf^\circ = 53.638 - 2.902\times10^{-3}T\ln T + 1.409\times10^{-6}T^2 + 437.975T^{-1} - 2.778\times10^{-3}T$

1945-2000 K: $\Delta Hf^\circ = 60.770 - 5.071\times10^{-3}T + 0.037\times10^{-6}T^2 + 107.850T^{-1}$

$\Delta Gf^\circ = 60.770 + 5.071\times10^{-3}T\ln T - 0.037\times10^{-6}T^2 + 53.925T^{-1} - 63.910\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

$TiI_2(c,g)$
Titanium Diiodide
[Formation: $Ti(c,l) + I_2(c,l,g) = TiI_2(c,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	20.609	29.300	29.300	0	-63.600	-61.877	45.357
300	20.612	29.428	29.301	.038	-63.597	-61.866	45.069
386.8	20.763	34.684	29.943	1.834	-63.542	-61.376	34.678
386.8	20.763	34.684	29.943	1.834	-67.251	-61.376	34.678
400	20.786	35.381	30.111	2.108	-67.315	-61.175	33.424
458.4	20.888	38.220	30.968	3.325	-67.597	-60.258	28.729
458.4	20.888	38.220	30.968	3.325	-77.618	-60.258	28.729
500	20.960	40.038	31.648	4.195	-77.389	-58.691	25.654
600	21.134	43.875	33.375	6.300	-76.845	-55.004	20.035
700	21.308	47.146	35.115	8.422	-76.311	-51.400	16.048
800	21.482	50.002	36.799	10.562	-75.785	-47.877	13.079
900	21.656	52.543	38.411	12.719	-75.270	-44.420	10.786
1000	21.830	54.833	39.940	14.893	-74.759	-41.017	8.964
1100	22.004	56.922	41.390	17.085	-74.257	-37.674	7.485
1156	22.101	58.017	42.169	18.320	-73.979	-35.816	6.771
1156	22.101	58.017	42.169	18.320	-74.996	-35.816	6.771
1200	22.178	58.844	42.766	19.294	-74.732	-34.329	6.252
1300	22.352	60.626	44.072	21.520	-74.136	-30.986	5.209
1358.2	22.453	61.606	44.805	22.820	-73.796	-29.065	4.677
1358.2	15.014	99.745	44.805	74.620	-21.996	-29.065	4.677
1400	15.037	100.199	46.451	75.247	-22.062	-29.280	4.571
1500	15.102	101.239	50.070	76.754	-22.228	-29.791	4.340
1600	15.177	102.216	53.299	78.268	-22.410	-30.288	4.137
1700	15.259	103.138	56.203	79.790	-22.610	-30.773	3.956
1800	15.348	104.013	58.835	81.320	-22.833	-31.250	3.794
1900	15.440	104.845	61.235	82.859	-23.085	-31.709	3.647
1945	15.483	105.207	62.248	83.555	-23.210	-31.913	3.586
1945	15.483	105.207	62.248	83.555	-26.510	-31.913	3.586
2000	15.535	105.640	63.436	84.408	-26.771	-32.063	3.504

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
1156 K, α - β transition point of Ti; $\Delta H°$ = 1.017 kcal/mol.
1358.2 K, sublimation point of TiI_2; $\Delta H°$ = 51.800 kcal/mol.
1945 K, melting point of Ti; $\Delta H°$ = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1358.2 K: $Cp° = 20.112 + 1.712\times10^{-3}T - 0.011\times10^{5}T^{-2}$

$H°- H°_{298} = 20.112\times10^{-3}T + 0.856\times10^{-6}T^{2} + 0.011\times10^{2}T^{-1} - 6.076$

1358.2-2000 K: $Cp° = 12.926 + 1.198\times10^{-3}T + 8.521\times10^{5}T^{-2}$

$H°- H°_{298} = 12.926\times10^{-3}T + 0.599\times10^{-6}T^{2} - 8.521\times10^{2}T^{-1} + 56.586$

TiI_2(c,g) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -63.922 + 1.758\times10^{-3}T - 1.759\times10^{-6}T^2 - 13.700T^{-1}$

$\Delta Gf^\circ = -63.922 - 1.758\times10^{-3}T\ln T + 1.759\times10^{-6}T^2 - 6.850T^{-1} + 16.426\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -65.377 - 4.646\times10^{-3}T - 0.267\times10^{-6}T^2 - 13.700T^{-1}$

$\Delta Gf^\circ = -65.377 + 4.646\times10^{-3}T\ln T + 0.267\times10^{-6}T^2 - 6.850T^{-1} - 17.389\times10^{-3}T$

458.4-1156 K: $\Delta Hf^\circ = -80.090 + 5.694\times10^{-3}T - 0.335\times10^{-6}T^2 - 29.000T^{-1}$

$\Delta Gf^\circ = -80.090 - 5.694\times10^{-3}T\ln T + 0.335\times10^{-6}T^2 - 14.500T^{-1} + 78.074\times10^{-3}T$

1156-1358.2 K: $\Delta Hf^\circ = -84.127 + 8.094\times10^{-3}T - 0.658\times10^{-6}T^2 + 753.900T^{-1}$

$\Delta Gf^\circ = -84.127 - 8.094\times10^{-3}T\ln T + 0.658\times10^{-6}T^2 + 376.950T^{-1} + 97.826\times10^{-3}T$

1358.2-1945 K: $\Delta Hf^\circ = -21.465 + 0.908\times10^{-3}T - 0.915\times10^{-6}T^2 - 99.300T^{-1}$

$\Delta Gf^\circ = -21.465 - 0.908\times10^{-3}T\ln T + 0.915\times10^{-6}T^2 - 49.650T^{-1} - 0.267\times10^{-3}T$

1945-2000 K: $\Delta Hf^\circ = -14.333 - 7.065\times10^{-3}T + 0.531\times10^{-6}T^2 - 867.400T^{-1}$

$\Delta Gf^\circ = -14.333 + 7.065\times10^{-3}T\ln T - 0.531\times10^{-6}T^2 - 433.700T^{-1} - 61.399\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$TiI_2(g)$

Titanium Diiodide (ideal gas)

[Formation: $Ti(c,l) + I_2(c,l,g) = TiI_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	14.476	77.335	77.335	0	-4.700	-17.299	12.680
300	14.481	77.425	77.335	.027	-4.708	-17.376	12.658
386.8	14.636	81.126	77.787	1.292	-5.184	-20.982	11.855
386.8	14.636	81.126	77.787	1.292	-8.893	-20.982	11.855
400	14.659	81.618	77.905	1.485	-9.038	-21.392	11.688
458.4	14.709	83.621	78.509	2.343	-9.678	-23.151	11.038
458.4	14.709	83.621	78.509	2.343	-19.699	-23.151	11.038
500	14.745	84.900	78.988	2.956	-19.728	-23.462	10.255
600	14.793	87.593	80.205	4.433	-19.812	-24.202	8.815
700	14.822	89.875	81.426	5.914	-19.919	-24.918	7.780
800	14.843	91.856	82.610	7.397	-20.050	-25.625	7.000
900	14.861	93.605	83.736	8.882	-20.207	-26.313	6.389
1000	14.880	95.172	84.803	10.369	-20.383	-26.980	5.896
1100	14.905	96.591	85.811	11.858	-20.584	-27.637	5.491
1156	14.924	97.331	86.351	12.693	-20.706	-27.990	5.292
1156	14.924	97.331	86.351	12.693	-21.723	-27.990	5.292
1200	14.939	97.889	86.764	13.350	-21.776	-28.227	5.141
1300	14.983	99.087	87.667	14.846	-21.910	-28.760	4.835
1400	15.037	100.199	88.523	16.347	-22.062	-29.280	4.571
1500	15.102	101.239	89.336	17.854	-22.228	-29.791	4.340
1600	15.177	102.216	90.111	19.368	-22.410	-30.288	4.137
1700	15.259	103.138	90.850	20.890	-22.610	-30.773	3.956
1800	15.348	104.013	91.557	22.420	-22.833	-31.250	3.794
1900	15.440	104.845	92.235	23.959	-23.085	-31.709	3.647
1945	15.483	105.207	92.531	24.655	-23.210	-31.913	3.586
1945	15.483	105.207	92.531	24.655	-26.510	-31.913	3.586
2000	15.535	105.640	92.886	25.508	-26.771	-32.063	3.504

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1945 K, melting point of Ti; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 14.697 + 0.268\times10^{-3}T - 0.267\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.697\times10^{-3}T + 0.134\times10^{-6}T^2 + 0.267\times10^{2}T^{-1} - 4.483$

$TiI_2(g)$ - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -3.429 - 3.657\times10^{-3}T - 2.481\times10^{-6}T^2 + 11.900T^{-1}$

$\Delta Gf^\circ = -3.429 + 3.657\times10^{-3}T\ln T + 2.481\times10^{-6}T^2 + 5.950T^{-1} - 68.163\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -4.884 - 10.061\times10^{-3}T - 0.989\times10^{-6}T^2 + 11.900T^{-1}$

$\Delta Gf^\circ = -4.884 + 10.061\times10^{-3}T\ln T + 0.989\times10^{-6}T^2 + 5.950T^{-1} - 101.978\times10^{-3}T$

458.4-1156 K: $\Delta Hf^\circ = -19.597 + 0.279\times10^{-3}T - 1.057\times10^{-6}T^2 - 3.400T^{-1}$

$\Delta Gf^\circ = -19.597 - 0.279\times10^{-3}T\ln T + 1.057\times10^{-6}T^2 - 1.700T^{-1} - 6.515\times10^{-3}T$

1156-1945 K: $\Delta Hf^\circ = -23.634 + 2.679\times10^{-3}T - 1.380\times10^{-6}T^2 + 779.500T^{-1}$

$\Delta Gf^\circ = -23.634 - 2.679\times10^{-3}T\ln T + 1.380\times10^{-6}T^2 + 389.750T^{-1} + 13.237\times10^{-3}T$

1945-2000 K: $\Delta Hf^\circ = -16.502 - 5.294\times10^{-3}T + 0.066\times10^{-6}T^2 + 11.400T^{-1}$

$\Delta Gf^\circ = -16.502 + 5.294\times10^{-3}T\ln T - 0.066\times10^{-6}T^2 + 5.700T^{-1} - 47.895\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

TiI_3(c,g)

Titanium Triiodide

[Formation: $Ti(c,l) + 1.5I_2(c,l,g) = TiI_3(c,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	27.910	45.500	45.500	0	-80.880	-79.849	58.530
300	27.910	45.673	45.500	.052	-80.875	-79.841	58.164
386.8	28.066	52.784	46.369	2.481	-80.791	-79.560	44.952
386.8	28.066	52.784	46.369	2.481	-86.354	-79.560	44.952
400	28.090	53.726	46.596	2.852	-86.449	-79.326	43.341
458.4	28.189	57.560	47.755	4.495	-86.867	-78.256	37.309
458.4	28.189	57.560	47.755	4.495	-101.898	-78.256	37.309
500	28.260	60.012	48.674	5.669	-101.552	-76.123	33.273
600	28.430	65.180	51.007	8.504	-100.727	-71.116	25.904
700	28.610	69.576	53.353	11.356	-99.912	-66.240	20.681
800	28.780	73.408	55.627	14.225	-99.107	-61.485	16.797
900	28.960	76.808	57.795	17.112	-98.314	-56.830	13.800
1000	29.130	79.868	59.852	20.016	-97.526	-52.261	11.422
1092	29.290	82.438	61.647	22.704	-96.809	-48.135	9.633
1092	20.613	117.705	61.647	61.216	-58.297	-48.135	9.633
1100	20.612	117.854	62.052	61.382	-58.304	-48.058	9.548
1156	20.605	118.877	64.780	62.537	-58.361	-47.531	8.986
1156	20.605	118.877	64.780	62.537	-59.378	-47.531	8.986
1200	20.599	119.647	66.778	63.443	-59.381	-47.080	8.574
1300	20.586	121.295	70.909	65.502	-59.406	-46.053	7.742
1400	20.574	122.820	74.563	67.560	-59.458	-45.023	7.028
1500	20.562	124.239	77.828	69.617	-59.530	-43.991	6.409
1600	20.551	125.566	80.771	71.672	-59.628	-42.951	5.867
1700	20.541	126.812	83.443	73.727	-59.753	-41.906	5.387
1800	20.530	127.986	85.885	75.781	-59.910	-40.853	4.960
1900	20.521	129.095	88.130	77.833	-60.109	-39.787	4.576
1945	20.517	129.575	89.084	78.756	-60.213	-39.305	4.416
1945	20.517	129.575	89.084	78.756	-63.513	-39.305	4.416
2000	20.512	130.148	90.205	79.885	-63.752	-38.618	4.220

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
1092 K, sublimation point of TiI_3; $\Delta H°$ = 38.512 kcal/mol.
1156 K, α - β transition point of Ti; $\Delta H°$ = 1.017 kcal/mol.
1945 K, melting point of Ti; $\Delta H°$ = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1092 K: $Cp° = 27.383 + 1.748\times10^{-3}T + 0.005\times10^{5}T^{-2}$

$H°- H°_{298} = 27.383\times10^{-3}T + 0.874\times10^{-6}T^{2} - 0.005\times10^{2}T^{-1} - 8.240$

1092-2000 K: $Cp° = 20.953 - 0.220\times10^{-3}T - 1.173\times10^{5}T^{-2}$

$H°- H°_{298} = 20.953\times10^{-3}T - 0.110\times10^{-6}T^{2} + 1.173\times10^{2}T^{-1} + 38.359$

TiI_3(c,g) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -81.380 + 2.590\times10^{-3}T - 2.487\times10^{-6}T^2 - 15.300T^{-1}$

$\Delta Gf^\circ = -81.380 - 2.590\times10^{-3}T\ln T + 2.487\times10^{-6}T^2 - 7.650T^{-1} + 19.238\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -83.563 - 7.016\times10^{-3}T - 0.249\times10^{-6}T^2 - 15.300T^{-1}$

$\Delta Gf^\circ = -83.563 + 7.016\times10^{-3}T\ln T + 0.249\times10^{-6}T^2 - 7.650T^{-1} - 31.485\times10^{-3}T$

458.4-1092 K: $\Delta Hf^\circ = -105.632 + 8.495\times10^{-3}T - 0.351\times10^{-6}T^2 - 38.250T^{-1}$

$\Delta Gf^\circ = -105.632 - 8.495\times10^{-3}T\ln T + 0.351\times10^{-6}T^2 - 19.125T^{-1} + 111.710\times10^{-3}T$

1092-1156 K: $\Delta Hf^\circ = -59.033 + 2.065\times10^{-3}T - 1.335\times10^{-6}T^2 + 79.550T^{-1}$

$\Delta Gf^\circ = -59.033 - 2.065\times10^{-3}T\ln T + 1.335\times10^{-6}T^2 + 39.775T^{-1} + 22.930\times10^{-3}T$

1156-1945 K: $\Delta Hf^\circ = -63.070 + 4.464\times10^{-3}T - 1.658\times10^{-6}T^2 + 862.450T^{-1}$

$\Delta Gf^\circ = -63.070 - 4.464\times10^{-3}T\ln T + 1.658\times10^{-6}T^2 + 431.225T^{-1} + 42.682\times10^{-3}T$

1945-2000 K: $\Delta Hf^\circ = -55.938 - 3.509\times10^{-3}T - 0.212\times10^{-6}T^2 + 94.350T^{-1}$

$\Delta Gf^\circ = -55.938 + 3.509\times10^{-3}T\ln T + 0.212\times10^{-6}T^2 + 47.175T^{-1} - 18.450\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Cartwright (21). Entropy at 298 K estimated. High-temperature data for crystal based on heat capacities estimated by Kelley (117). Gas data are those estimated by JANAF (60).

$TiI_3(g)$

Titanium Triiodide (ideal gas)

[Formation: $Ti(c,l) + 1.5I_2(c,l,g) = TiI_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	19.311	91.294	91.294	0	-35.900	-48.523	35.568
300	19.332	91.414	91.294	.036	-35.911	-48.600	35.404
386.8	19.983	96.420	91.904	1.747	-36.545	-52.193	29.490
386.8	19.983	96.420	91.904	1.747	-42.109	-52.193	29.490
400	20.082	97.092	92.065	2.011	-42.310	-52.534	28.703
458.4	20.279	99.847	92.883	3.192	-43.189	-53.963	25.727
458.4	20.279	99.847	92.883	3.192	-58.221	-53.963	25.727
500	20.420	101.615	93.537	4.039	-58.202	-53.575	23.417
600	20.569	105.353	95.205	6.089	-58.162	-52.655	19.179
700	20.627	108.529	96.886	8.150	-58.138	-51.733	16.151
800	20.641	111.284	98.518	10.213	-58.140	-50.818	13.883
900	20.637	113.715	100.074	12.277	-58.170	-49.902	12.118
1000	20.625	115.889	101.549	14.340	-58.222	-48.979	10.704
1100	20.612	117.854	102.943	16.402	-58.304	-48.058	9.548
1156	20.605	118.877	103.690	17.557	-58.361	-47.531	8.986
1156	20.605	118.877	103.690	17.557	-59.378	-47.531	8.986
1200	20.599	119.647	104.261	18.463	-59.381	-47.080	8.574
1300	20.586	121.295	105.509	20.522	-59.407	-46.053	7.742
1400	20.574	122.820	106.691	22.580	-59.458	-45.023	7.028
1500	20.562	124.239	107.814	24.637	-59.530	-43.991	6.409
1600	20.551	125.566	108.883	26.692	-59.628	-42.951	5.867
1700	20.541	126.812	109.902	28.747	-59.753	-41.906	5.387
1800	20.530	127.986	110.874	30.801	-59.911	-40.853	4.960
1900	20.521	129.095	111.804	32.853	-60.109	-39.787	4.576
1945	20.517	129.575	112.210	33.776	-60.213	-39.305	4.416
1945	20.517	129.575	112.210	33.776	-63.513	-39.305	4.416
2000	20.512	130.148	112.695	34.905	-63.752	-38.618	4.220

*Data estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1945 K, melting point of Ti; ΔH° = 3.300 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 21.255 - 0.424\times10^{-3}T - 1.616\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 21.255\times10^{-3}T - 0.212\times10^{-6}T^2 + 1.616\times10^{2}T^{-1} - 6.860$

$TiI_3(g)$ - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -35.020 - 3.538\times10^{-3}T - 3.573\times10^{-6}T^2 + 146.800T^{-1}$

$\Delta Gf^\circ = -35.020 + 3.538\times10^{-3}T\ln T + 3.573\times10^{-6}T^2 + 73.400T^{-1} - 67.335\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -37.203 - 13.144\times10^{-3}T - 1.335\times10^{-6}T^2 + 146.800T^{-1}$

$\Delta Gf^\circ = -37.203 + 13.144\times10^{-3}T\ln T + 1.335\times10^{-6}T^2 + 73.400T^{-1} - 118.058\times10^{-3}T$

458.4-1156 K: $\Delta Hf^\circ = -59.273 + 2.366\times10^{-3}T - 1.437\times10^{-6}T^2 + 123.850T^{-1}$

$\Delta Gf^\circ = -59.273 - 2.366\times10^{-3}T\ln T + 1.437\times10^{-6}T^2 + 61.925T^{-1} + 25.137\times10^{-3}T$

1156-1945 K: $\Delta Hf^\circ = -63.310 + 4.766\times10^{-3}T - 1.760\times10^{-6}T^2 + 906.750T^{-1}$

$\Delta Gf^\circ = -63.310 - 4.766\times10^{-3}T\ln T + 1.760\times10^{-6}T^2 + 453.375T^{-1} + 44.889\times10^{-3}T$

1945-2000 K: $\Delta Hf^\circ = -56.177 - 3.207\times10^{-3}T - 0.314\times10^{-6}T^2 + 138.650T^{-1}$

$\Delta Gf^\circ = -56.177 + 3.207\times10^{-3}T\ln T + 0.314\times10^{-6}T^2 + 69.325T^{-1} - 16.243\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

$TiI_4(c,l,g)$

Titanium Tetraiodide

[Formation: $Ti(c,l) + 2I_2(c,l,g) = TiI_4(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	30.030	58.830	58.830	0	-89.800	-88.606	64.949
300	30.081	59.016	58.830	.056	-89.803	-88.596	64.542
379	34.066	66.439	59.658	2.570	-89.954	-88.261	50.895
379	45.900	72.389	59.658	4.825	-87.699	-88.261	50.895
386.8	45.900	73.324	59.924	5.183	-87.625	-88.273	49.875
386.8	45.900	73.324	59.924	5.183	-95.043	-88.273	49.875
400	45.900	74.864	60.391	5.789	-95.030	-88.042	48.103
428	45.900	77.970	61.440	7.075	-95.001	-87.553	44.707
428	37.500	87.877	61.440	11.315	-90.761	-87.553	44.707
458.4	37.500	90.450	63.280	12.455	-90.987	-87.315	41.628
458.4	37.500	90.450	63.280	12.455	-111.029	-87.315	41.628
500	37.500	93.708	65.678	14.015	-110.483	-85.184	37.233
600	37.500	100.545	70.937	17.765	-109.191	-80.248	29.230
651.3	37.500	103.622	73.390	19.690	-108.538	-77.793	26.104
651.3*	25.628	123.290	73.390	32.500	-95.728	-77.793	26.104
700	25.658	125.142	76.929	33.749	-95.694	-76.455	23.870
800	25.698	128.571	83.175	36.317	-95.641	-73.711	20.137
900	25.727	131.599	88.389	38.889	-95.615	-70.970	17.234
1000	25.747	134.311	92.849	41.462	-95.610	-68.231	14.912
1100	25.762	136.766	96.731	44.038	-95.631	-65.500	13.013
1156	25.768	138.045	98.702	45.481	-95.654	-63.962	12.092
1156	25.768	138.045	98.702	45.481	-96.671	-63.962	12.092
1200	25.773	139.008	100.162	46.615	-96.647	-62.717	11.422
1300	25.782	141.071	103.231	49.192	-96.609	-59.890	10.068
1400	25.789	142.982	106.003	51.771	-96.595	-57.066	8.908
1500	25.795	144.761	108.528	54.350	-96.602	-54.244	7.903
1600	25.799	146.426	110.845	56.930	-96.632	-51.416	7.023
1700	25.803	147.990	112.984	59.510	-96.690	-48.589	6.246
1800	25.806	149.465	114.971	62.090	-96.780	-45.759	5.556
1900	25.809	150.861	116.824	64.671	-96.909	-42.920	4.937
1945	25.810	151.465	117.618	65.832	-96.982	-41.642	4.679
1945	25.810	151.465	117.618	65.832	-100.282	-41.642	4.679
2000	25.811	152.185	118.559	67.252	-100.483	-39.981	4.369

*Data for gas estimated.

Phase changes: 379 K, α - β transition point of TiI_4; ΔH° = 2.255 kcal/mol.
386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
428 K, melting point of TiI_4; ΔH° = 4.240 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
651.3 K, boiling point of TiI_4; ΔH° = 12.810 kcal/mol.
1156 K, α - β transition point of Ti; ΔH° = 1.017 kcal/mol.
1945 K, melting point of Ti; ΔH° = 3.300 kcal/mol.

TiI_4(c,l,g) - Continued

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-379 K: $Cp^\circ = 17.069 + 43.468\times10^{-3}T$

$H^\circ - H^\circ_{298} = 17.069\times10^{-3}T + 21.734\times10^{-6}T^2 - 7.021$

379-428 K: $Cp^\circ = 45.901$

$H^\circ - H^\circ_{298} = 45.901\times10^{-3}T - 12.571$

428-651.3 K: $Cp^\circ = 37.500$

$H^\circ - H^\circ_{298} = 37.500\times10^{-3}T - 4.735$

651.3-2000 K: $Cp^\circ = 25.887 - 0.034\times10^{-3}T - 1.009\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.887\times10^{-3}T - 0.017\times10^{-6}T^2 + 1.009\times10^{2}T^{-1} + 15.492$

Formation equations (kcal/mol):

298.15-379 K: $\Delta Hf^\circ = -87.095 - 14.162\times10^{-3}T + 17.627\times10^{-6}T^2 - 14.800T^{-1}$

$\Delta Gf^\circ = -87.095 + 14.162\times10^{-3}T\ln T - 17.627\times10^{-6}T^2 - 7.400T^{-1} - 80.418\times10^{-3}T$

379-386.8 K: $\Delta Hf^\circ = -92.645 + 14.670\times10^{-3}T - 4.107\times10^{-6}T^2 - 14.800T^{-1}$

$\Delta Gf^\circ = -92.645 - 14.670\times10^{-3}T\ln T + 4.107\times10^{-6}T^2 - 7.400T^{-1} + 97.181\times10^{-3}T$

386.8-428 K: $\Delta Hf^\circ = -95.556 + 1.862\times10^{-3}T - 1.123\times10^{-6}T^2 - 14.800T^{-1}$

$\Delta Gf^\circ = -95.556 - 1.862\times10^{-3}T\ln T + 1.123\times10^{-6}T^2 - 7.400T^{-1} + 29.551\times10^{-3}T$

428-458.4 K: $\Delta Hf^\circ = -87.720 - 6.539\times10^{-3}T - 1.123\times10^{-6}T^2 - 14.800T^{-1}$

$\Delta Gf^\circ = -87.720 + 6.539\times10^{-3}T\ln T + 1.123\times10^{-6}T^2 - 7.400T^{-1} - 39.660\times10^{-3}T$

458.4-651.3 K: $\Delta Hf^\circ = -117.146 + 14.141\times10^{-3}T - 1.259\times10^{-6}T^2 - 45.400T^{-1}$

$\Delta Gf^\circ = -117.146 - 14.141\times10^{-3}T\ln T + 1.259\times10^{-6}T^2 - 22.700T^{-1} + 151.266\times10^{-3}T$

651.3-1156 K: $\Delta Hf^\circ = -96.921 + 2.528\times10^{-3}T - 1.276\times10^{-6}T^2 + 55.500T^{-1}$

$\Delta Gf^\circ = -96.921 - 2.528\times10^{-3}T\ln T + 1.276\times10^{-6}T^2 + 27.750T^{-1} + 44.841\times10^{-3}T$

1156-1945 K: $\Delta Hf^\circ = -100.958 + 4.928\times10^{-3}T - 1.599\times10^{-6}T^2 + 838.400T^{-1}$

$\Delta Gf^\circ = -100.958 - 4.928\times10^{-3}T\ln T + 1.599\times10^{-6}T^2 + 419.200T^{-1} + 64.594\times10^{-3}T$

1945-2000 K: $\Delta Hf^\circ = -93.825 - 3.045\times10^{-3}T - 0.153\times10^{-6}T^2 + 70.300T^{-1}$

$\Delta Gf^\circ = -93.825 + 3.045\times10^{-3}T\ln T + 0.153\times10^{-6}T^2 + 35.150T^{-1} + 3.461\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (254). Low-temperature heat capacities and entropy at 298 K from King (129). High-temperature data for crystal and liquid based on King (129). Gas data are those estimated by JANAF (60).

$TiI_4(g)$
Titanium Tetraiodide (ideal gas)
[Formation: $Ti(c,l) + 2I_2(c,l,g) = TiI_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	24.917	103.479	103.479	0	-66.270	-78.388	57.459
300	24.928	103.633	103.480	.046	-66.283	-78.461	57.158
386.8	25.259	110.016	104.260	2.226	-67.052	-81.892	46.270
386.8	25.259	110.016	104.260	2.226	-74.470	-81.892	46.270
400	25.309	110.864	104.464	2.560	-74.729	-82.141	44.879
458.4	25.416	114.322	105.502	4.043	-75.869	-83.140	39.638
458.4	25.416	114.322	105.502	4.043	-95.911	-83.140	39.638
500	25.493	116.533	106.329	5.102	-95.866	-81.979	35.833
600	25.595	121.191	108.429	7.657	-95.769	-79.213	28.853
700	25.658	125.142	110.543	10.219	-95.694	-76.455	23.870
800	25.698	128.571	112.587	12.787	-95.641	-73.711	20.137
900	25.727	131.599	114.533	15.359	-95.615	-70.970	17.234
1000	25.747	134.311	116.379	17.932	-95.610	-68.231	14.912
1100	25.762	136.766	118.122	20.508	-95.631	-65.500	13.013
1156	25.768	138.045	119.056	21.951	-95.654	-63.962	12.092
1156	25.768	138.045	119.056	21.951	-96.671	-63.962	12.092
1200	25.773	139.008	119.771	23.085	-96.647	-62.717	11.422
1300	25.782	141.071	121.331	25.662	-96.609	-59.890	10.068
1400	25.789	142.982	122.810	28.241	-96.595	-57.066	8.908
1500	25.795	144.761	124.214	30.820	-96.602	-54.243	7.903
1600	25.799	146.426	125.551	33.400	-96.632	-51.416	7.023
1700	25.803	147.990	126.825	35.980	-96.690	-48.589	6.246
1800	25.806	149.465	128.043	38.560	-96.780	-45.759	5.556
1900	25.809	150.861	129.208	41.141	-96.909	-42.920	4.937
1945	25.810	151.465	129.716	42.302	-96.982	-41.642	4.679
1945	25.810	151.465	129.716	42.302	-100.282	-41.642	4.679
2000	25.811	152.185	130.324	43.722	-100.483	-39.981	4.369

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; $\Delta H° = 3.709$ kcal/mol.
458.4 K, boiling point of I_2; $\Delta H° = 10.021$ kcal/mol.
1156 K, α - β transition point of Ti; $\Delta H° = 1.017$ kcal/mol.
1945 K, melting point of Ti; $\Delta H° = 3.300$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 25.806 + 0.016\times10^{-3}T - 0.795\times10^{5}T^{-2}$

$H°- H°_{298} = 25.806\times10^{-3}T + 0.008\times10^{-6}T^{2} + 0.795\times10^{2}T^{-1} - 7.961$

TiI_4(g) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -64.505 - 5.425\times10^{-3}T - 4.099\times10^{-6}T^2 + 64.700T^{-1}$

$\Delta Gf^\circ = -64.505 + 5.425\times10^{-3}T\ln T + 4.099\times10^{-6}T^2 + 32.350T^{-1} - 79.058\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -67.415 - 18.233\times10^{-3}T - 1.115\times10^{-6}T^2 + 64.700T^{-1}$

$\Delta Gf^\circ = -67.415 + 18.233\times10^{-3}T\ln T + 1.115\times10^{-6}T^2 + 32.350T^{-1} - 146.688\times10^{-3}T$

458.4-1156 K: $\Delta Hf^\circ = -96.842 + 2.447\times10^{-3}T - 1.251\times10^{-6}T^2 + 34.100T^{-1}$

$\Delta Gf^\circ = -96.842 - 2.447\times10^{-3}T\ln T + 1.251\times10^{-6}T^2 + 17.050T^{-1} + 44.237\times10^{-3}T$

1156-1945 K: $\Delta Hf^\circ = -100.879 + 4.847\times10^{-3}T - 1.574\times10^{-6}T^2 + 817.000T^{-1}$

$\Delta Gf^\circ = -100.879 - 4.847\times10^{-3}T\ln T + 1.574\times10^{-6}T^2 + 408.500T^{-1} + 63.990\times10^{-3}T$

1945-2000 K: $\Delta Hf^\circ = -93.747 - 3.126\times10^{-3}T - 0.128\times10^{-6}T^2 + 48.900T^{-1}$

$\Delta Gf^\circ = -93.747 + 3.126\times10^{-3}T\ln T + 0.128\times10^{-6}T^2 + 24.450T^{-1} + 2.857\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

TlBr(c,l)

Thallium Bromide

[Formation: $Tl(c,l) + 0.5Br_2(l,g) = TlBr(c,l)$

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.550	29.300	29.300	0	-41.400	-40.139	29.422
300	12.554	29.380	29.303	.023	-41.406	-40.132	29.236
332.6	12.631	30.679	29.376	.434	-41.496	-39.989	26.276
332.6	12.631	30.679	29.376	.434	-45.028	-39.989	26.276
400	12.790	32.960	29.785	1.270	-44.921	-38.977	21.296
500	13.500	35.890	30.720	2.585	-44.724	-37.513	16.396
507	13.550	36.078	30.793	2.680	-44.710	-37.411	16.126
507	13.550	36.078	30.793	2.680	-44.800	-37.411	16.126
577	14.047	37.858	31.541	3.645	-44.686	-36.396	13.786
577	14.047	37.858	31.541	3.645	-45.676	-36.396	13.786
600	14.210	38.410	31.793	3.970	-45.617	-36.027	13.123
700	14.920	40.660	32.910	5.425	-45.318	-34.454	10.757
733.2	15.160	41.350	33.276	5.920	-45.207	-33.942	10.117
733.2	18.620	46.700	33.279	9.840	-41.287	-33.942	10.117
800	18.020	48.300	34.463	11.070	-40.831	-33.296	9.096
900	17.110	50.360	36.110	12.825	-40.235	-32.381	7.863
1000	16.210	52.130	37.640	14.490	-39.730	-31.549	6.895
1100	15.310	53.630	39.021	16.070	-39.311	-30.741	6.108
1200	14.400	54.920	40.291	17.555	-38.988	-29.983	5.461

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
507 K, α - β transition point of Tl; ΔH° = 0.090 kcal/mol.
577 K, melting point of Tl; ΔH° = 0.990 kcal/mol.
733.2 K, melting point of TlBr; ΔH° = 3.920 kcal/mol.
1100 ± 10 K, boiling point of TlBr to equilibrium mixture of monomer and dimer. Enthalpy of sublimation to monomer at 298 K = 32.5 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-733.2 K: $Cp^\circ = 9.950 + 7.094\times10^{-3}T$

$H^\circ - H^\circ_{298} = 9.950\times10^{-3}T + 3.547\times10^{-6}T^2 - 3.282$

733.2-1200 K: $Cp^\circ = 25.251 - 9.040\times10^{-3}T$

$H^\circ - H^\circ_{298} = 25.251\times10^{-3}T - 4.520\times10^{-6}T^2 - 6.244$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -40.730 - 3.122\times10^{-3}T + 0.847\times10^{-6}T^2 + 55.400T^{-1}$

$\Delta Gf^\circ = -40.730 + 3.122\times10^{-3}T\ln T - 0.847\times10^{-6}T^2 + 27.700T^{-1} - 15.860\times10^{-3}T$

332.6-507 K: $\Delta Hf^\circ = -45.731 + 1.459\times10^{-3}T + 0.770\times10^{-6}T^2 + 39.700T^{-1}$

$\Delta Gf^\circ = -45.731 - 1.459\times10^{-3}T\ln T - 0.770\times10^{-6}T^2 + 19.850T^{-1} + 25.817\times10^{-3}T$

507-577 K: $\Delta Hf^\circ = -44.875 - 1.006\times10^{-3}T + 2.377\times10^{-6}T^2 - 15.700T^{-1}$

$\Delta Gf^\circ = -44.875 + 1.006\times10^{-3}T\ln T - 2.377\times10^{-6}T^2 - 7.850T^{-1} + 9.698\times10^{-3}T$

577-733.2 K: $\Delta Hf^\circ = -45.894 - 1.615\times10^{-3}T + 3.520\times10^{-6}T^2 - 15.700T^{-1}$

$\Delta Gf^\circ = -45.894 + 1.615\times10^{-3}T\ln T - 3.520\times10^{-6}T^2 - 7.850T^{-1} + 8.252\times10^{-3}T$

733.2-1200 K: $\Delta Hf^\circ = -48.856 + 13.686\times10^{-3}T - 4.547\times10^{-6}T^2 - 15.700T^{-1}$

$\Delta Gf^\circ = -48.856 - 13.686\times10^{-3}T\ln T + 4.547\times10^{-6}T^2 - 7.850T^{-1} + 107.324\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Low-temperature heat capacities and entropy at 298 K from Takahashi (234). High-temperature data from Cubicciotti (49). Vaporization data from Cubicciotti (41).

TlCl(c,l)
Thallium Chloride
[Formation: $Tl(c,l) + 0.5Cl_2(g) = TlCl(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	12.170	26.590	26.590	0	-48.790	-44.200	32.399
300	12.180	26.670	26.593	.023	-48.787	-44.173	32.179
400	12.640	30.250	27.075	1.270	-48.596	-42.663	23.309
500	13.100	33.120	28.020	2.550	-48.419	-41.207	18.011
507	13.138	33.302	28.092	2.642	-48.407	-41.105	17.719
507	13.138	33.302	28.092	2.642	-48.497	-41.105	17.719
577	13.516	35.019	28.819	3.578	-48.406	-40.084	15.182
577	13.516	35.019	28.819	3.578	-49.396	-40.084	15.182
600	13.640	35.550	29.067	3.890	-49.348	-39.714	14.465
700	14.020	37.680	30.166	5.260	-49.127	-38.134	11.906
704	14.040	37.780	30.221	5.320	-49.113	-38.080	11.821
704	17.900	43.060	30.221	9.040	-45.393	-38.080	11.821
800	17.900	45.350	31.900	10.760	-44.780	-37.128	10.143
900	17.900	47.460	33.516	12.550	-44.145	-36.208	8.792
1000	17.900	49.340	35.000	14.340	-43.512	-35.353	7.726
1100	17.900	51.050	36.386	16.130	-42.880	-34.568	6.868
1200	17.900	52.610	37.677	17.920	-42.250	-33.852	6.165

Phase changes: 507 K, α - β transition point of Tl; $\Delta H°$ = 0.090 kcal/mol.
577 K, melting point of Tl; $\Delta H°$ = 0.990 kcal/mol.
704 K, melting point of TlCl; $\Delta H°$ = 3.720 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-704 K:
$$Cp° = 10.801 + 4.604\times10^{-3}T$$
$$H°- H°_{298} = 10.801\times10^{-3}T + 2.302\times10^{-6}T^2 - 3.425$$

704-1200 K:
$$Cp° = 17.900$$
$$H°- H°_{298} = 17.900\times10^{-3}T - 3.562$$

Formation equations (kcal/mol):

298.15-507 K:
$$\Delta Hf° = -49.522 + 2.361\times10^{-3}T - 0.492\times10^{-6}T^2 + 21.250T^{-1}$$
$$\Delta Gf° = -49.522 - 2.361\times10^{-3}T\ln T + 0.492\times10^{-6}T^2 + 10.625T^{-1} + 31.038\times10^{-3}T$$

507-577 K:
$$\Delta Hf° = -48.666 - 0.104\times10^{-3}T + 1.115\times10^{-6}T^2 - 34.150T^{-1}$$
$$\Delta Gf° = -48.666 + 0.104\times10^{-3}T\ln T - 1.115\times10^{-6}T^2 - 17.075T^{-1} + 14.919\times10^{-3}T$$

577-704 K:
$$\Delta Hf° = -49.685 - 0.713\times10^{-3}T + 2.258\times10^{-6}T^2 - 34.150T^{-1}$$
$$\Delta Gf° = -49.685 + 0.713\times10^{-3}T\ln T - 2.258\times10^{-6}T^2 - 17.075T^{-1} + 13.472\times10^{-3}T$$

704-1200 K:
$$\Delta Hf° = -49.822 + 6.386\times10^{-3}T - 0.044\times10^{-6}T^2 - 34.150T^{-1}$$
$$\Delta Gf° = -49.822 - 6.386\times10^{-3}T\ln T + 0.044\times10^{-6}T^2 - 17.075T^{-1} + 58.593\times10^{-3}T$$

Sources: Enthalpy of formation at 298 K from Wagman (252). Low-temperature heat capacities and entropy at 298 K from Bartky (9). High-temperature data based on Eding (71).

TlCl(g)

Thallium Chloride (ideal gas)

[Formation: $Tl(c,l) + 0.5Cl_2(g) = TlCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.660	61.220	61.220	0	-16.120	-21.855	16.020
300	8.670	61.280	61.227	.016	-16.124	-21.893	15.948
400	8.780	63.790	61.568	.889	-16.307	-23.790	12.998
500	8.840	65.760	62.220	1.770	-16.529	-25.637	11.206
507	8.842	65.883	62.270	1.832	-16.547	-25.764	11.106
507	8.842	65.883	62.270	1.832	-16.637	-25.764	11.106
577	8.863	67.023	62.774	2.452	-16.862	-27.006	10.229
577	8.863	67.023	62.774	2.452	-17.852	-27.006	10.229
600	8.870	67.370	62.943	2.656	-17.912	-27.370	9.969
700	8.890	68.740	63.677	3.544	-18.173	-28.922	9.030
800	8.900	69.920	64.379	4.433	-18.437	-30.441	8.316
900	8.910	70.970	65.054	5.324	-18.701	-31.923	7.752
1000	8.920	71.910	65.695	6.215	-18.967	-33.378	7.295
1100	8.920	72.760	66.299	7.107	-19.233	-34.802	6.914
1200	8.920	73.540	66.874	7.999	-19.501	-36.219	6.596
1300	8.920	74.250	67.411	8.891	-19.770	-37.594	6.320
1400	8.930	74.910	67.921	9.784	-20.039	-38.947	6.080
1500	8.930	75.530	68.411	10.678	-20.308	-40.293	5.871

Phase changes: 507 K, α - β transition point of Tl; $\Delta H° = 0.090$ kcal/mol.
577 K, melting point of Tl; $\Delta H° = 0.990$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 8.938 - 0.245\times10^{5}T^{-2}$

$H°- H°_{298} = 8.938\times10^{-3}T + 0.245\times10^{2}T^{-1} - 2.747$

Formation equations (kcal/mol):

298.15-507 K: $\Delta Hf° = -16.174 + 0.498\times10^{-3}T - 2.794\times10^{-6}T^{2} + 45.750T^{-1}$

$\Delta Gf° = -16.174 - 0.498\times10^{-3}T\ln T + 2.794\times10^{-6}T^{2} + 22.875T^{-1} - 17.305\times10^{-3}T$

507-577 K: $\Delta Hf° = -15.318 - 1.967\times10^{-3}T - 1.187\times10^{-6}T^{2} - 9.650T^{-1}$

$\Delta Gf° = -15.318 + 1.967\times10^{-3}T\ln T + 1.187\times10^{-6}T^{2} - 4.825T^{-1} - 33.424\times10^{-3}T$

577-1500 K: $\Delta Hf° = -16.337 - 2.576\times10^{-3}T - 0.044\times10^{-6}T^{2} - 9.650T^{-1}$

$\Delta Gf° = -16.337 + 2.576\times10^{-3}T\ln T + 0.044\times10^{-6}T^{2} - 4.825T^{-1} - 34.870\times10^{-3}T$

Source: Data from Drapcho (64).

$(TlCl)_2(g)$

Dimeric Thallium Chloride (ideal gas)

[Formation: $2Tl(c,l) + Cl_2(g) = (TlCl)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.390	92.440	92.440	0	-57.100	-59.625	43.706
300	19.400	92.560	92.440	.036	-57.103	-59.641	43.448
400	19.600	98.170	93.202	1.987	-57.264	-60.466	33.037
500	19.700	102.550	94.646	3.952	-57.506	-61.236	26.766
507	19.704	102.824	94.757	4.090	-57.528	-61.286	26.418
507	19.704	102.824	94.757	4.090	-57.708	-61.286	26.418
577	19.739	105.378	95.897	5.471	-58.017	-61.764	23.394
577	19.739	105.378	95.897	5.471	-59.997	-61.764	23.394
600	19.750	106.150	96.275	5.925	-60.070	-61.832	22.522
700	19.780	109.200	97.911	7.902	-60.391	-62.095	19.387
800	19.800	111.840	99.489	9.881	-60.718	-62.328	17.027
900	19.820	114.170	100.990	11.862	-61.047	-62.499	15.177
1000	19.830	116.260	102.416	13.844	-61.379	-62.641	13.690
1100	19.830	118.150	103.762	15.827	-61.713	-62.744	12.466
1200	19.840	119.880	105.037	17.811	-62.049	-62.846	11.446
1300	19.840	121.470	106.243	19.795	-62.387	-62.897	10.574
1400	19.850	122.940	107.383	21.780	-62.726	-62.911	9.821
1500	19.850	124.310	108.467	23.765	-63.067	-62.912	9.166

Phase changes: 507 K, α - β transition point of Tl; $\Delta H° = 0.090$ kcal/mol.
577 K, melting point of Tl; $\Delta H° = 0.990$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 19.863 + 0.006\times10^{-3}T - 0.422\times10^{5}T^{-2}$

$H°- H°_{298} = 19.863\times10^{-3}T + 0.003\times10^{-6}T^2 + 0.422\times10^{2}T^{-1} - 6.064$

Formation equations (kcal/mol):

298.15-507 K: $\Delta Hf° = -57.777 + 2.984\times10^{-3}T - 5.585\times10^{-6}T^2 + 84.700T^{-1}$

$\Delta Gf° = -57.777 - 2.984\times10^{-3}T\ln T + 5.585\times10^{-6}T^2 + 42.350T^{-1} + 8.662\times10^{-3}T$

507-577 K: $\Delta Hf° = -56.065 - 1.946\times10^{-3}T - 2.371\times10^{-6}T^2 - 26.100T^{-1}$

$\Delta Gf° = -56.065 + 1.946\times10^{-3}T\ln T + 2.371\times10^{-6}T^2 - 13.050T^{-1} - 23.576\times10^{-3}T$

577-1500 K: $\Delta Hf° = -58.104 - 3.164\times10^{-3}T - 0.085\times10^{-6}T^2 - 26.100T^{-1}$

$\Delta Gf° = -58.104 + 3.164\times10^{-3}T\ln T + 0.085\times10^{-6}T^2 - 13.050T^{-1} - 26.469\times10^{-3}T$

Source: Data from Drapcho (64).

TlF(c,l)
Thallium Fluoride
[Formation: $Tl(c,l) + 0.5F_2(g) = TlF(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	12.760	22.870	22.870	0	-77.600	-72.623	53.234
300	12.780	22.950	22.873	.023	-77.596	-72.594	52.884
356.3	200.000	25.200	23.059	.762	-77.428	-71.667	43.959
356.3	12.820	25.420	23.059	.842	-77.348	-71.667	43.959
400	13.190	26.930	23.405	1.410	-77.234	-70.978	38.780
500	14.180	29.890	24.470	2.710	-77.013	-69.470	30.365
507	14.305	30.088	24.546	2.810	-76.992	-69.364	29.900
507	14.305	30.088	24.546	2.810	-77.082	-69.364	29.900
577	15.552	32.007	25.333	3.851	-76.872	-68.310	25.873
577	15.552	32.007	25.333	3.851	-77.862	-68.310	25.873
595.4	15.880	32.500	25.549	4.140	-77.781	-68.008	24.963
595.4	16.080	38.080	25.549	7.460	-74.461	-68.008	24.963
600	16.080	38.200	25.642	7.535	-74.438	-67.956	24.753
700	16.080	40.680	27.623	9.140	-73.966	-66.913	20.891
800	16.080	42.830	29.393	10.750	-73.497	-65.945	18.015
900	16.080	44.720	30.987	12.360	-73.033	-65.019	15.789
1000	16.080	46.420	32.455	13.965	-72.578	-64.160	14.022
1100	16.080	47.950	33.791	15.575	-72.121	-63.332	12.583
1200	16.080	49.350	35.033	17.180	-71.672	-62.566	11.395

Phase changes: 356.3 K, α - β transition point of TlF; $\Delta H°$ = 0.080 kcal/mol.
507 K, α - β transition point of Tl; $\Delta H°$ = 0.090 kcal/mol.
577 K, melting point of Tl; $\Delta H°$ = 0.990 kcal/mol.
595.4 K, melting point of TlF; $\Delta H°$ = 3.320 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-356.3 K: $Cp° = 9.232 + 11.828\times10^{-3}T$
$H°- H°_{298} = 9.232\times10^{-3}T + 5.914\times10^{-6}T^2 - 3.278$

356.3-595.4 K: $Cp° = 9.907 + 8.160\times10^{-3}T + 0.007\times10^{5}T^{-2}$
$H°- H°_{298} = 9.907\times10^{-3}T + 4.080\times10^{-6}T^2 - 0.007\times10^{2}T^{-1} - 3.204$

595.4-1200 K: $Cp° = 16.080$
$H°- H°_{298} = 16.080\times10^{-3}T - 2.114$

Formation equations (kcal/mol):

298.15-356.3 K: $\Delta Hf° = -78.175 + 0.952\times10^{-3}T + 3.077\times10^{-6}T^2 + 5.150T^{-1}$
$\Delta Gf° = -78.175 - 0.952\times10^{-3}T\ln T - 3.077\times10^{-6}T^2 + 2.575T^{-1} + 24.931\times10^{-3}T$

356.3-507 K: $\Delta Hf° = -78.100 + 1.627\times10^{-3}T + 1.243\times10^{-6}T^2 + 4.450T^{-1}$
$\Delta Gf° = -78.100 - 1.627\times10^{-3}T\ln T - 1.243\times10^{-6}T^2 + 2.225T^{-1} + 28.038\times10^{-3}T$

507-577 K: $\Delta Hf° = -77.244 - 0.838\times10^{-3}T + 2.850\times10^{-6}T^2 - 50.950T^{-1}$
$\Delta Gf° = -77.244 + 0.838\times10^{-3}T\ln T - 2.850\times10^{-6}T^2 - 25.475T^{-1} + 11.919\times10^{-3}T$

577-595.4 K: $\Delta Hf° = -78.264 - 1.447\times10^{-3}T + 3.993\times10^{-6}T^2 - 50.950T^{-1}$
$\Delta Gf° = -78.264 + 1.447\times10^{-3}T\ln T - 3.993\times10^{-6}T^2 - 25.475T^{-1} + 10.473\times10^{-3}T$

595.4-1200 K: $\Delta Hf° = -77.174 + 4.726\times10^{-3}T - 0.087\times10^{-6}T^2 - 50.250T^{-1}$
$\Delta Gf° = -77.174 - 4.726\times10^{-3}T\ln T + 0.087\times10^{-6}T^2 - 25.125T^{-1} + 45.653\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Low-temperature heat capacities, entropy at 298 K, and data to 400 K from Lyon (148). High-temperature data above 400 K based on Cubicciotti (49).

TlF(g)

Thallium Fluoride (ideal gas)

[Formation: $Tl(c,l,g) + 0.5F_2(g) = TlF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	8.293	58.431	58.431	0	-44.420	-50.046	36.684
300	8.300	58.483	58.433	.015	-44.424	-50.082	36.484
400	8.568	60.911	58.761	.860	-44.604	-51.941	28.379
500	8.718	62.840	59.390	1.725	-44.819	-53.750	23.494
507	8.725	62.961	59.438	1.786	-44.836	-53.875	23.223
507	8.725	62.961	59.438	1.786	-44.926	-53.875	23.223
577	8.791	64.095	59.936	2.400	-45.144	-55.096	20.868
577	8.791	64.095	59.936	2.400	-46.134	-55.096	20.868
600	8.813	64.439	60.102	2.602	-46.190	-55.452	20.198
700	8.877	65.802	60.822	3.486	-46.440	-56.973	17.787
800	8.924	66.991	61.520	4.377	-46.690	-58.466	15.972
900	8.962	68.044	62.187	5.271	-46.942	-59.920	14.550
1000	8.993	68.990	62.821	6.169	-47.194	-61.346	13.407
1100	9.020	69.849	63.422	7.070	-47.446	-62.746	12.466
1200	9.045	70.635	63.991	7.973	-47.698	-64.136	11.681
1300	9.067	71.360	64.531	8.878	-47.951	-65.493	11.010
1400	9.088	72.032	65.042	9.786	-48.203	-66.827	10.432
1500	9.109	72.660	65.529	10.696	-48.454	-68.149	9.929
1600	9.129	73.248	65.993	11.608	-48.706	-69.450	9.486
1700	9.149	73.802	66.436	12.522	-48.956	-70.738	9.094
1746	9.158	74.046	66.633	12.943	-49.071	-71.326	8.928
1746	9.158	74.046	66.633	12.943	-88.286	-71.326	8.928
1800	9.168	74.326	66.860	13.438	-88.320	-70.795	8.596
1900	9.188	74.822	67.267	14.355	-88.390	-69.819	8.031
2000	9.208	75.293	67.656	15.275	-88.465	-68.837	7.522

Phase changes: 507 K, α - β transition point of Tl; $\Delta H° = 0.090$ kcal/mol.
577 K, melting point of Tl; $\Delta H° = 0.990$ kcal/mol.
1746 K, boiling point of Tl; $\Delta H° = 39.215$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.849 + 0.190\times10^{-3}T - 0.545\times10^{5}T^{-2}$

$H°- H°_{298} = 8.849\times10^{-3}T + 0.095\times10^{-6}T^{2} + 0.545\times10^{2}T^{-1} - 2.830$

Formation equations (kcal/mol):

298.15-507 K: $\Delta Hf° = -44.546 + 0.569\times10^{-3}T - 2.742\times10^{-6}T^{2} + 59.650T^{-1}$

$\Delta Gf° = -44.546 - 0.569\times10^{-3}T\ln T + 2.742\times10^{-6}T^{2} + 29.825T^{-1} - 16.358\times10^{-3}T$

507-577 K: $\Delta Hf° = -43.690 - 1.896\times10^{-3}T - 1.135\times10^{-6}T^{2} + 4.250T^{-1}$

$\Delta Gf° = -43.690 + 1.896\times10^{-3}T\ln T + 1.135\times10^{-6}T^{2} + 2.125T^{-1} - 32.477\times10^{-3}T$

577-1746 K: $\Delta Hf° = -44.709 - 2.505\times10^{-3}T + 0.008\times10^{-6}T^{2} + 4.250T^{-1}$

$\Delta Gf° = -44.709 + 2.505\times10^{-3}T\ln T - 0.008\times10^{-6}T^{2} + 2.125T^{-1} - 33.923\times10^{-3}T$

1746-2000 K: $\Delta Hf° = -87.184 - 0.568\times10^{-3}T - 0.032\times10^{-6}T^{2} + 4.250T^{-1}$

$\Delta Gf° = -87.184 + 0.568\times10^{-3}T\ln T + 0.032\times10^{-6}T^{2} + 2.125T^{-1} + 4.794\times10^{-3}T$

Source: Data from Gurvich (95).

$(TlF)_2(g)$

Dimeric Thallium Fluoride (ideal gas)

[Formation: $2Tl(c,l,g) + F_2(g) = (TlF)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.739	85.533	85.533	0	-122.800	-124.711	91.415
300	18.752	85.649	85.533	.035	-122.803	-124.723	90.859
400	19.218	91.116	86.276	1.936	-122.953	-125.343	68.484
500	19.446	95.431	87.689	3.871	-123.176	-125.915	55.037
507	19.455	95.701	87.798	4.007	-123.197	-125.951	54.292
507	19.455	95.701	87.798	4.007	-123.377	-125.951	54.292
577	19.544	98.225	88.914	5.372	-123.674	-126.290	47.834
577	19.544	98.225	88.914	5.372	-125.654	-126.290	47.834
600	19.573	98.989	89.286	5.822	-125.723	-126.313	46.009
700	19.651	102.012	90.892	7.784	-126.029	-126.379	39.457
800	19.702	104.640	92.450	9.752	-126.343	-126.421	34.536
900	19.738	106.963	93.936	11.724	-126.662	-126.405	30.695
1000	19.763	109.044	95.345	13.699	-126.987	-126.356	27.615
1100	19.782	110.928	96.677	15.676	-127.316	-126.269	25.087
1200	19.796	112.650	97.938	17.655	-127.648	-126.178	22.980
1300	19.807	114.235	99.131	19.635	-127.983	-126.037	21.188
1400	19.816	115.703	100.263	21.616	-128.322	-125.865	19.648
1500	19.823	117.071	101.339	23.598	-128.663	-125.678	18.311
1600	19.829	118.350	102.362	25.581	-129.006	-125.460	17.137
1700	19.834	119.553	103.339	27.564	-129.351	-125.230	16.099
1746	19.836	120.083	103.773	28.476	-129.512	-125.116	15.661
1746	19.836	120.083	103.773	28.476	-207.942	-125.116	15.661
1800	19.838	120.686	104.270	29.548	-207.927	-122.539	14.878
1900	19.842	121.759	105.163	31.532	-207.918	-117.795	13.549
2000	19.844	122.777	106.019	33.516	-207.925	-113.051	12.353

Phase changes: 507 K, α - β transition point of Tl; $\Delta H°$ = 0.090 kcal/mol.
577 K, melting point of Tl; $\Delta H°$ = 0.990 kcal/mol.
1746 K, boiling point of Tl; $\Delta H°$ = 39.215 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.826 + 0.028\times10^{-3}T - 0.974\times10^{5}T^{-2}$

$H°- H°_{298} = 19.826\times10^{-3}T + 0.014\times10^{-6}T^2 + 0.974\times10^{2}T^{-1} - 6.239$

Formation equations (kcal/mol):

298.15-507 K: $\Delta Hf° = -123.632 + 3.266\times10^{-3}T - 5.660\times10^{-6}T^2 + 107.700T^{-1}$

$\Delta Gf° = -123.632 - 3.266\times10^{-3}T\ln T + 5.660\times10^{-6}T^2 + 53.850T^{-1} + 12.695\times10^{-3}T$

507-577 K: $\Delta Hf° = -121.920 - 1.664\times10^{-3}T - 2.446\times10^{-6}T^2 - 3.100T^{-1}$

$\Delta Gf° = -121.920 + 1.664\times10^{-3}T\ln T + 2.446\times10^{-6}T^2 - 1.550T^{-1} - 19.543\times10^{-3}T$

577-1746 K: $\Delta Hf° = -123.958 - 2.882\times10^{-3}T - 0.160\times10^{-6}T^2 - 3.100T^{-1}$

$\Delta Gf° = -123.958 + 2.882\times10^{-3}T\ln T + 0.160\times10^{-6}T^2 - 1.550T^{-1} - 22.435\times10^{-3}T$

1746-2000 K: $\Delta Hf° = -208.908 + 0.992\times10^{-3}T - 0.240\times10^{-6}T^2 - 3.100T^{-1}$

$\Delta Gf° = -208.908 - 0.992\times10^{-3}T\ln T + 0.240\times10^{-6}T^2 - 1.550T^{-1} + 54.999\times10^{-3}T$

Source: Data from Gurvich (95).

TlI(c,l)
Thallium Iodide
[Formation: $Tl(c,l) + 0.5I_2(c,l,g) = TlI(c,l)$

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	12.740	30.520	30.520	0	-29.600	-29.988	21.981
300	12.750	30.600	30.523	.023	-29.601	-29.991	21.848
386.8	12.872	33.828	30.919	1.125	-29.658	-30.100	17.007
386.8	12.872	33.828	30.919	1.125	-31.512	-30.100	17.007
400	12.890	34.260	31.022	1.295	-31.556	-30.052	16.419
451	13.060	35.820	31.479	1.957	-31.723	-29.848	14.464
451	12.800	36.300	31.479	2.175	-31.505	-29.848	14.464
458.4	12.883	36.509	31.557	2.270	-31.532	-29.820	14.217
458.4	12.883	36.509	31.557	2.270	-36.543	-29.820	14.217
500	13.350	37.650	32.010	2.820	-36.467	-29.209	12.767
507	13.429	37.836	32.089	2.914	-36.455	-29.107	12.547
507	13.429	37.836	32.089	2.914	-36.545	-29.107	12.547
577	14.220	39.629	32.905	3.880	-36.433	-28.092	10.640
577	14.220	39.629	32.905	3.880	-37.423	-28.092	10.640
600	14.480	40.190	33.173	4.210	-37.360	-27.721	10.097
700	15.600	42.500	34.343	5.710	-37.019	-26.136	8.160
714.8	15.770	42.830	34.514	5.945	-36.956	-25.906	7.921
714.8	17.200	47.750	34.514	9.460	-33.441	-25.906	7.921
800	17.200	49.680	36.024	10.925	-32.965	-25.038	6.840
900	17.200	51.710	37.660	12.645	-32.407	-24.081	5.848
1000	17.200	53.520	39.155	14.365	-31.849	-23.182	5.066
1100	17.200	55.160	40.537	16.085	-31.293	-22.339	4.438
1200	17.200	56.660	41.823	17.805	-30.737	-21.563	3.927

Phase changes: 386.8 K, melting point of I_2; $\Delta H° = 3.709$ kcal/mol.
451 K, α - β transition point of TlI; $\Delta H° = 0.218$ kcal/mol.
458.4 K, boiling point of I_2; $\Delta H° = 10.021$ kcal/mol.
507 K, α - β transition point of Tl; $\Delta H° = 0.090$ kcal/mol.
577 K, melting point of Tl; $\Delta H° = 0.990$ kcal/mol.
714.8 K, melting point of TlI; $\Delta H° = 3.515$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-451 K: $Cp° = 11.560 + 3.320\times10^{-3}T$
$H°- H°_{298} = 11.560\times10^{-3}T + 1.660\times10^{-6}T^2 - 3.594$

451-714.8 K: $Cp° = 7.721 + 11.268\times10^{-3}T$
$H°- H°_{298} = 7.721\times10^{-3}T + 5.634\times10^{-6}T^2 - 2.453$

714.8-1200 K: $Cp° = 17.200$
$H°- H°_{298} = 17.200\times10^{-3}T - 2.835$

TlI(c,l) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -29.949 + 1.096\times10^{-3}T - 1.836\times10^{-6}T^2 + 55.400T^{-1}$

$\Delta Gf^\circ = -29.949 - 1.096\times10^{-3}T\ln T + 1.836\times10^{-6}T^2 + 27.700T^{-1} + 5.253\times10^{-3}T$

386.8-451 K: $\Delta Hf^\circ = -30.677 - 2.106\times10^{-3}T - 1.090\times10^{-6}T^2 + 55.400T^{-1}$

$\Delta Gf^\circ = -30.677 + 2.106\times10^{-3}T\ln T + 1.090\times10^{-6}T^2 + 27.700T^{-1} - 11.655\times10^{-3}T$

451-458.4 K: $\Delta Hf^\circ = -29.536 - 5.945\times10^{-3}T + 2.884\times10^{-6}T^2 + 55.400T^{-1}$

$\Delta Gf^\circ = -29.536 + 5.945\times10^{-3}T\ln T - 2.884\times10^{-6}T^2 + 27.700T^{-1} - 35.854\times10^{-3}T$

458.4-507 K: $\Delta Hf^\circ = -36.892 - 0.776\times10^{-3}T + 2.850\times10^{-6}T^2 + 47.750T^{-1}$

$\Delta Gf^\circ = -36.892 + 0.776\times10^{-3}T\ln T - 2.850\times10^{-6}T^2 + 23.875T^{-1} + 11.877\times10^{-3}T$

507-577 K: $\Delta Hf^\circ = -36.036 - 3.241\times10^{-3}T + 4.457\times10^{-6}T^2 - 7.650T^{-1}$

$\Delta Gf^\circ = -36.036 + 3.241\times10^{-3}T\ln T - 4.457\times10^{-6}T^2 - 3.825T^{-1} - 4.242\times10^{-3}T$

577-714.8 K: $\Delta Hf^\circ = -37.056 - 3.849\times10^{-3}T + 5.600\times10^{-6}T^2 - 7.650T^{-1}$

$\Delta Gf^\circ = -37.056 + 3.849\times10^{-3}T\ln T - 5.600\times10^{-6}T^2 - 3.825T^{-1} - 5.688\times10^{-3}T$

714.8-1200 K: $\Delta Hf^\circ = -37.437 + 5.630\times10^{-3}T - 0.034\times10^{-6}T^2 - 7.650T^{-1}$

$\Delta Gf^\circ = -37.437 - 5.630\times10^{-3}T\ln T + 0.034\times10^{-6}T^2 - 3.825T^{-1} + 53.115\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Low-temperature heat capacities and entropy at 298 K from Takahashi (234). High-temperature data based on Cubicciotti (49).

$TmBr_3(g)$

Thulium Tribromide (ideal gas)

[Formation: $Tm(c,l) + 1.5Br_2(l,g) = TmBr_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.082	95.862	95.862	0	-130.400	-137.437	100.743
300	19.091	95.981	95.864	.035	-130.426	-137.481	100.153
332.6	19.198	97.956	95.974	.659	-130.895	-138.224	90.825
332.6	19.198	97.956	95.974	.659	-141.493	-138.224	90.825
400	19.418	101.524	96.617	1.963	-141.509	-137.565	75.161
500	19.577	105.876	98.048	3.914	-141.531	-136.576	59.697
600	19.666	109.454	99.661	5.876	-141.554	-135.583	49.386
700	19.720	112.489	101.280	7.846	-141.590	-134.582	42.018
800	19.755	115.125	102.851	9.819	-141.651	-133.580	36.492
900	19.779	117.453	104.346	11.796	-141.743	-132.565	32.191
1000	19.797	119.538	105.763	13.775	-141.859	-131.534	28.746
1100	19.810	121.426	107.103	15.755	-141.994	-130.502	25.928
1200	19.820	123.150	108.369	17.737	-142.146	-129.448	23.575
1300	19.827	124.737	109.569	19.719	-142.320	-128.383	21.583
1400	19.833	126.206	110.705	21.702	-142.512	-127.294	19.871
1500	19.838	127.575	111.784	23.686	-142.724	-126.209	18.388
1600	19.842	128.855	112.811	25.670	-142.956	-125.099	17.087
1700	19.846	130.058	113.791	27.654	-143.206	-123.972	15.937
1800	19.849	131.193	114.727	29.639	-143.472	-122.843	14.915
1818	19.849	131.391	114.891	29.996	-143.522	-122.630	14.742
1818	19.849	131.391	114.891	29.996	-147.547	-122.630	14.742
1900	19.851	132.266	115.622	31.624	-147.852	-121.502	13.976
2000	19.853	133.284	116.479	33.609	-148.245	-120.120	13.126

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.
1818 K, melting point of Tm; $\Delta H° = 4.025$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.840 + 0.020\times10^{-3}T - 0.679\times10^{5}T^{-2}$

$H°- H°_{298} = 19.840\times10^{-3}T + 0.010\times10^{-6}T^2 + 0.679\times10^{2}T^{-1} - 6.144$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -126.944 - 12.618\times10^{-3}T - 0.874\times10^{-6}T^2 + 114.300T^{-1}$

$\Delta Gf° = -126.944 + 12.618\times10^{-3}T\ln T + 0.874\times10^{-6}T^2 + 57.150T^{-1} - 107.989\times10^{-3}T$

332.6-1818 K: $\Delta Hf° = -141.944 + 1.124\times10^{-3}T - 1.107\times10^{-6}T^2 + 67.200T^{-1}$

$\Delta Gf° = -141.944 - 1.124\times10^{-3}T\ln T + 1.107\times10^{-6}T^2 + 33.600T^{-1} + 17.044\times10^{-3}T$

1818-2000 K: $\Delta Hf° = -141.055 - 3.445\times10^{-3}T - 0.072\times10^{-6}T^2 + 20.800T^{-1}$

$\Delta Gf° = -141.055 + 3.445\times10^{-3}T\ln T + 0.072\times10^{-6}T^2 + 10.400T^{-1} - 15.851\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166) and Kim (122). Other data based on Myers (165) and Dieke (56).

$TmCl_3(g)$

Thulium Trichloride (ideal gas)

[Formation: $Tm(c,l) + 1.5Cl_2(g) = TmCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	18.664	89.392	89.392	0	-159.100	-156.645	114.823
300	18.677	89.507	89.392	.035	-159.100	-156.630	114.103
400	19.165	94.956	90.131	1.930	-159.098	-155.809	85.129
500	19.409	99.261	91.541	3.860	-159.097	-154.986	67.743
600	19.546	102.813	93.133	5.808	-159.106	-154.164	56.153
700	19.631	105.833	94.737	7.767	-159.130	-153.336	47.873
800	19.686	108.458	96.292	9.733	-159.185	-152.509	41.663
900	19.725	110.779	97.775	11.704	-159.269	-151.667	36.829
1000	19.752	112.859	99.181	13.678	-159.381	-150.813	32.960
1100	19.773	114.743	100.512	15.654	-159.512	-149.957	29.793
1200	19.789	116.464	101.771	17.632	-159.664	-149.080	27.151
1300	19.801	118.048	102.962	19.612	-159.835	-148.188	24.912
1400	19.811	119.516	104.093	21.592	-160.027	-147.279	22.991
1500	19.818	120.883	105.167	23.574	-160.238	-146.368	21.326
1600	19.825	122.162	106.190	25.556	-160.470	-145.436	19.865
1700	19.830	123.364	107.165	27.539	-160.720	-144.480	18.574
1800	19.835	124.498	108.097	29.522	-160.988	-143.531	17.427
1818	19.836	124.695	108.260	29.879	-161.038	-143.348	17.232
1818	19.836	124.695	108.260	29.879	-165.063	-143.348	17.232
1900	19.839	125.570	108.988	31.506	-165.369	-142.365	16.375
2000	19.842	126.588	109.843	33.490	-165.765	-141.158	15.425

Phase change: 1818 K, melting point of Tm; ΔH° = 4.025 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.809 + 0.038\times10^{-3}T - 1.028\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.809\times10^{-3}T + 0.019\times10^{-6}T^2 + 1.028\times10^{2}T^{-1} - 6.253$

Formation equations (kcal/mol):

298.15-1818 K: $\Delta Hf^\circ = -159.527 + 1.248\times10^{-3}T - 1.147\times10^{-6}T^2 + 46.750T^{-1}$

$\Delta Gf^\circ = -159.527 - 1.248\times10^{-3}T\ln T + 1.147\times10^{-6}T^2 + 23.375T^{-1} + 16.167\times10^{-3}T$

1818-2000 K: $\Delta Hf^\circ = -158.637 - 3.322\times10^{-3}T - 0.113\times10^{-6}T^2 + 0.350T^{-1}$

$\Delta Gf^\circ = -158.637 + 3.322\times10^{-3}T\ln T + 0.113\times10^{-6}T^2 + 0.175T^{-1} - 16.728\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166) and Schumm (207). Other data based on Myers (165) and Dieke (56).

$TmF_3(c,l)$
Thulium Trifluoride
[Formation: $Tm(c,l) + 1.5F_2(g) = TmF_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	22.700	27.600	27.600	0	-395.800	-377.090	276.411
300	22.722	27.740	27.600	.042	-395.791	-376.974	274.622
400	23.690	34.419	28.504	2.366	-395.268	-370.780	202.582
500	24.370	39.782	30.240	4.771	-394.719	-364.721	159.417
600	24.891	44.274	32.216	7.235	-394.154	-358.775	130.682
700	25.309	48.143	34.222	9.745	-393.581	-352.922	110.186
800	25.657	51.546	36.179	12.294	-393.017	-347.156	94.837
900	25.959	54.586	38.058	14.875	-392.463	-341.453	82.915
1000	26.238	57.335	39.850	17.485	-391.918	-335.810	73.390
1100	26.511	59.849	41.555	20.123	-391.371	-330.232	65.610
1200	26.800	62.168	43.178	22.788	-390.823	-324.697	59.135
1300	27.120	64.325	44.722	25.484	-390.267	-319.205	53.663
1326	27.211	64.863	45.112	26.190	-390.122	-317.786	52.376
1326	23.390	70.323	45.112	33.430	-382.882	-317.786	52.376
1400	23.390	71.593	46.479	35.160	-382.757	-314.151	49.041
1431	23.390	72.105	47.028	35.885	-382.708	-312.633	47.746
1431	33.540	76.927	47.028	42.785	-375.808	-312.633	47.746
1500	33.540	78.506	48.440	45.099	-375.007	-309.613	45.110
1600	33.540	80.671	50.388	48.453	-373.863	-305.291	41.700
1700	33.540	82.704	52.229	51.807	-372.740	-301.032	38.700
1800	33.540	84.621	53.976	55.161	-371.639	-296.857	36.043
1818	33.540	84.955	54.281	55.765	-371.443	-296.102	35.595
1818	33.540	84.955	54.281	55.765	-375.468	-296.102	35.595
1900	33.540	86.435	55.638	58.515	-374.652	-292.547	33.650
2000	33.540	88.155	57.221	61.869	-373.681	-288.264	31.500

*Entropy and heat capacity at 298 K estimated.

Phase changes: 1326 K, α - β transition point of TmF_3; ΔH° = 7.240 kcal/mol.
1431 K, melting point of TmF_3; ΔH° = 6.900 kcal/mol.
1818 K, melting point of Tm; ΔH° = 4.025 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1326 K: $Cp^\circ = 23.649 + 2.744\times10^{-3}T - 1.573\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 23.649\times10^{-3}T + 1.372\times10^{-6}T^2 + 1.573\times10^{2}T^{-1} - 7.700$

1326-1431 K: $Cp^\circ = 23.385$

$H^\circ - H^\circ_{298} = 23.385\times10^{-3}T + 2.421$

1431-2000 K: $Cp^\circ = 33.541$

$H^\circ - H^\circ_{298} = 33.541\times10^{-3}T - 5.212$

TmF_3(c,l) - Continued

Formation equations (kcal/mol):

298.15-1326 K: $\Delta Hf^\circ = -397.644 + 5.566\times10^{-3}T + 0.077\times10^{-6}T^2 + 52.950T^{-1}$

$\Delta Gf^\circ = -397.644 - 5.566\times10^{-3}T\ln T - 0.077\times10^{-6}T^2 + 26.475T^{-1} + 100.377\times10^{-3}T$

1326-1431 K: $\Delta Hf^\circ = -387.523 + 5.302\times10^{-3}T - 1.295\times10^{-6}T^2 - 104.350T^{-1}$

$\Delta Gf^\circ = -387.523 - 5.302\times10^{-3}T\ln T + 1.295\times10^{-6}T^2 - 52.175T^{-1} + 89.072\times10^{-3}T$

1431-1818 K: $\Delta Hf^\circ = -395.156 + 15.458\times10^{-3}T - 1.295\times10^{-6}T^2 - 104.350T^{-1}$

$\Delta Gf^\circ = -395.156 - 15.458\times10^{-3}T\ln T + 1.295\times10^{-6}T^2 - 52.175T^{-1} + 168.201\times10^{-3}T$

1818-2000 K: $\Delta Hf^\circ = -394.267 + 10.889\times10^{-3}T - 0.261\times10^{-6}T^2 - 150.750T^{-1}$

$\Delta Gf^\circ = -394.267 - 10.889\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 - 75.375T^{-1} + 135.306\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Kim (121). Entropy and heat capacity at 298 K estimated. High-temperature data based on Spedding (222).

$TmF_3(g)$

Thulium Trifluoride (ideal gas)

[Formation: $Tm(c,l) + 1.5F_2(g) = TmF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	16.937	81.085	81.085	0	-290.600	-287.836	210.987
300	16.963	81.190	81.087	.031	-290.602	-287.820	209.674
400	17.997	86.226	81.766	1.784	-290.651	-286.885	156.745
500	18.588	90.311	83.079	3.616	-290.674	-285.940	124.983
600	18.946	93.734	84.577	5.494	-290.695	-284.992	103.807
700	19.175	96.673	86.100	7.401	-290.725	-284.037	88.679
800	19.330	99.244	87.585	9.327	-290.785	-283.081	77.333
900	19.439	101.528	89.010	11.266	-290.872	-282.110	68.505
1000	19.519	103.580	90.366	13.214	-290.989	-281.127	61.439
1100	19.579	105.444	91.654	15.169	-291.125	-280.140	55.658
1200	19.624	107.149	92.875	17.129	-291.282	-279.133	50.836
1300	19.660	108.721	94.034	19.093	-291.458	-278.111	46.754
1400	19.689	110.179	95.135	21.061	-291.656	-277.071	43.252
1500	19.712	111.539	96.185	23.031	-291.875	-276.031	40.217
1600	19.731	112.811	97.184	25.003	-292.114	-274.965	37.558
1700	19.747	114.008	98.139	26.977	-292.371	-273.879	35.209
1800	19.760	115.137	99.052	28.953	-292.647	-272.793	33.121
1818	19.762	115.334	99.212	29.309	-292.699	-272.588	32.769
1818	19.762	115.334	99.212	29.309	-296.724	-272.588	32.769
1900	19.772	116.206	99.928	30.929	-297.038	-271.498	31.229
2000	19.782	117.220	100.767	32.907	-297.443	-270.156	29.521

Phase change: 1818 K, melting point of Tm; $\Delta H° = 4.025$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.419 + 0.264\times10^{-3}T - 2.277\times10^{5}T^{-2}$

$H°-H°_{298} = 19.419\times10^{-3}T + 0.132\times10^{-6}T^2 + 2.277\times10^{2}T^{-1} - 6.565$

Formation equations (kcal/mol):

298.15-1818 K: $\Delta Hf° = -291.309 + 1.336\times10^{-3}T - 1.163\times10^{-6}T^2 + 123.350T^{-1}$

$\Delta Gf° = -291.309 - 1.336\times10^{-3}T\ln T + 1.163\times10^{-6}T^2 + 61.675T^{-1} + 18.218\times10^{-3}T$

1818-2000 K: $\Delta Hf° = -290.419 - 3.233\times10^{-3}T - 0.129\times10^{-6}T^2 + 76.950T^{-1}$

$\Delta Gf° = -290.419 + 3.233\times10^{-3}T\ln T + 0.129\times10^{-6}T^2 + 38.475T^{-1} - 14.677\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

$TmI_3(g)$

Thulium Triiodide (ideal gas)

[Formation: $Tm(c,l) + 1.5I_2(c,l,g) = TmI_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	19.464	102.697	102.697	0	-78.800	-91.731	67.240
300	19.469	102.817	102.697	.036	-78.812	-91.811	66.883
386.8	19.618	107.786	103.304	1.734	-79.488	-95.489	53.953
386.8	19.618	107.786	103.304	1.734	-85.052	-95.489	53.953
400	19.641	108.445	103.463	1.993	-85.261	-95.842	52.365
458.4	19.689	111.125	104.273	3.141	-86.180	-97.320	46.398
458.4	19.689	111.125	104.273	3.141	-101.211	-97.320	46.398
500	19.723	112.837	104.915	3.961	-101.220	-96.964	42.382
600	19.768	116.438	106.545	5.936	-101.244	-96.112	35.008
700	19.796	119.487	108.180	7.915	-101.279	-95.250	29.738
800	19.813	122.132	109.763	9.895	-101.343	-94.388	25.785
900	19.826	124.466	111.269	11.877	-101.437	-93.512	22.707
1000	19.834	126.556	112.696	13.860	-101.556	-92.619	20.242
1100	19.841	128.446	114.042	15.844	-101.695	-91.726	18.224
1200	19.846	130.173	115.316	17.828	-101.854	-90.812	16.539
1300	19.850	131.761	116.520	19.813	-102.031	-89.881	15.110
1400	19.853	133.233	117.663	21.798	-102.230	-88.932	13.883
1500	19.855	134.602	118.747	23.783	-102.448	-87.984	12.819
1600	19.857	135.884	119.778	25.769	-102.685	-87.010	11.885
1700	19.859	137.088	120.762	27.755	-102.942	-86.018	11.058
1800	19.860	138.223	121.700	29.741	-103.217	-85.025	10.323
1818	19.860	138.421	121.865	30.098	-103.268	-84.836	10.198
1818	19.860	138.421	121.865	30.098	-107.293	-84.836	10.198
1900	19.862	139.297	122.599	31.727	-107.606	-83.822	9.642
2000	19.863	140.316	123.459	33.713	-108.007	-82.573	9.023

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
1818 K, melting point of Tm; $\Delta H°$ = 4.025 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.863 + 0.006\times10^{-3}T - 0.357\times10^{5}T^{-2}$

$H°- H°_{298} = 19.863\times10^{-3}T + 0.003\times10^{-6}T^2 + 0.357\times10^{2}T^{-1} - 6.042$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -77.362 - 4.773\times10^{-3}T - 3.269\times10^{-6}T^2 + 82.100T^{-1}$

$\Delta Gf° = -77.362 + 4.773\times10^{-3}T\ln T + 3.269\times10^{-6}T^2 + 41.050T^{-1} - 76.828\times10^{-3}T$

386.8-458.4 K: $\Delta Hf° = -79.544 - 14.380\times10^{-3}T - 1.031\times10^{-6}T^2 + 82.100T^{-1}$

$\Delta Gf° = -79.544 + 14.380\times10^{-3}T\ln T + 1.031\times10^{-6}T^2 + 41.050T^{-1} - 127.551\times10^{-3}T$

458.4-1818 K: $\Delta Hf° = -101.614 + 1.131\times10^{-3}T - 1.133\times10^{-6}T^2 + 59.150T^{-1}$

$\Delta Gf° = -101.614 - 1.131\times10^{-3}T\ln T + 1.133\times10^{-6}T^2 + 29.575T^{-1} + 15.643\times10^{-3}T$

1818-2000 K: $\Delta Hf° = -100.725 - 3.439\times10^{-3}T - 0.099\times10^{-6}T^2 + 12.750T^{-1}$

$\Delta Gf° = -100.725 + 3.439\times10^{-3}T\ln T + 0.099\times10^{-6}T^2 + 6.375T^{-1} - 17.252\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166) and Schumm (207). Other data based on Myers (156) and Dieke (56).

$UBr_3(c)$
Uranium Tribromide
[Formation: $U(c) + 1.5Br_2(l,g) = UBr_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	25.980	46.000	46.000	0	-167.100	-160.968	117.991
300	25.990	46.160	46.000	.048	-167.113	-160.928	117.235
332.6	26.195	48.852	46.150	.899	-167.363	-160.244	105.294
332.6	26.195	48.852	46.150	.899	-177.961	-160.244	105.294
400	26.620	53.720	47.023	2.679	-177.532	-156.698	85.615
500	27.250	59.730	48.986	5.372	-176.898	-151.565	66.248
600	27.880	64.760	51.212	8.129	-176.270	-146.559	53.384
700	28.510	69.100	53.460	10.948	-175.658	-141.653	44.225
800	29.140	72.950	55.661	13.831	-175.071	-136.836	37.381
900	29.770	76.420	57.780	16.776	-174.523	-132.093	32.076
942	30.035	77.784	58.642	18.032	-174.307	-130.118	30.188
942	30.035	77.784	58.642	18.032	-174.974	-130.118	30.188
1000	30.400	79.590	59.805	19.785	-174.599	-127.368	27.836

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 24.110 + 6.286\times10^{-3}T - 0.003\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 24.110\times10^{-3}T + 3.143\times10^{-6}T^2 + 0.003\times10^{2}T^{-1} - 7.469$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -165.482 - 6.136\times10^{-3}T - 0.929\times10^{-6}T^2 + 87.800T^{-1}$

$\Delta Gf^\circ = -165.482 + 6.136\times10^{-3}T\ln T + 0.929\times10^{-6}T^2 + 43.900T^{-1} - 20.591\times10^{-3}T$

332.6-942 K: $\Delta Hf^\circ = -180.483 + 7.605\times10^{-3}T - 1.161\times10^{-6}T^2 + 40.700T^{-1}$

$\Delta Gf^\circ = -180.483 - 7.605\times10^{-3}T\ln T + 1.161\times10^{-6}T^2 + 20.350T^{-1} + 104.441\times10^{-3}T$

942-1000 K: $\Delta Hf^\circ = -178.073 + 0.460\times10^{-3}T + 3.060\times10^{-6}T^2 - 46.800T^{-1}$

$\Delta Gf^\circ = -178.073 - 0.460\times10^{-3}T\ln T - 3.060\times10^{-6}T^2 - 23.400T^{-1} + 56.980\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data are those estimations from Parker (186).

$UBr_4(c,l)$
Uranium Tetrabromide
[Formation: $U(c) + 2Br_2(l,g) = UBr_4(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	30.620	57.000	57.000	0	-191.800	-183.524	134.525
300	30.630	57.190	57.000	.057	-191.821	-183.471	133.657
332.6	30.861	60.362	57.177	1.059	-192.213	-182.544	119.947
332.6	30.861	60.362	57.177	1.059	-206.343	-182.544	119.947
400	31.340	66.100	58.212	3.155	-205.893	-177.772	97.129
500	32.050	73.170	60.520	6.325	-205.223	-170.819	74.664
600	32.760	79.070	63.128	9.565	-204.556	-163.997	59.735
700	33.470	84.180	65.784	12.877	-203.898	-157.293	49.108
792	34.120	88.350	68.167	15.986	-203.309	-151.204	41.724
792	41.000	103.000	68.167	27.586	-191.709	-151.204	41.724
800	41.000	103.410	68.518	27.914	-191.604	-150.795	41.195
900	41.000	108.240	72.669	32.014	-190.351	-145.772	35.398
942	41.000	110.110	74.297	33.736	-189.858	-143.704	33.340
942	41.000	110.110	74.297	33.736	-190.525	-143.704	33.340
1000	41.000	112.560	76.446	36.114	-189.786	-140.844	30.781
1040	41.000	114.170	77.868	37.754	-189.277	-138.897	29.188

*Entropy at 298 K and all heat capacities estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
792 K, melting point of UBr_4; ΔH° = 11.600 kcal/mol.
942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1040 K, boiling point of UBr_3; ΔH° (vap, 298 K) = 50 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-792 K: $Cp^\circ = 28.481 + 7.126\times10^{-3}T + 0.013\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 28.481\times10^{-3}T + 3.563\times10^{-6}T^2 - 0.013\times10^{2}T^{-1} - 8.804$

792-1040 K: $Cp^\circ = 41.000$

$H^\circ - H^\circ_{298} = 41.000\times10^{-3}T - 4.886$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -188.825 - 10.811\times10^{-3}T - 0.459\times10^{-6}T^2 + 86.200T^{-1}$

$\Delta Gf^\circ = -188.825 + 10.811\times10^{-3}T\ln T + 0.459\times10^{-6}T^2 + 43.100T^{-1} - 44.439\times10^{-3}T$

332.6-792 K: $\Delta Hf^\circ = -208.826 + 7.511\times10^{-3}T - 0.769\times10^{-6}T^2 + 23.400T^{-1}$

$\Delta Gf^\circ = -208.826 - 7.511\times10^{-3}T\ln T + 0.769\times10^{-6}T^2 + 11.700T^{-1} + 122.272\times10^{-3}T$

792-942 K: $\Delta Hf^\circ = -204.908 + 20.030\times10^{-3}T - 4.332\times10^{-6}T^2 + 24.700T^{-1}$

$\Delta Gf^\circ = -204.908 - 20.030\times10^{-3}T\ln T + 4.332\times10^{-6}T^2 + 12.350T^{-1} + 198.060\times10^{-3}T$

942-1040 K: $\Delta Hf^\circ = -202.498 + 12.885\times10^{-3}T - 0.110\times10^{-6}T^2 - 62.800T^{-1}$

$\Delta Gf^\circ = -202.498 - 12.885\times10^{-3}T\ln T + 0.110\times10^{-6}T^2 - 31.400T^{-1} + 150.599\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data from Parker (186). Who estimated all except temperature and enthalpy of fusion and vaporization data.

$UCl_3(c)$

Uranium Trichloride

[Formation: $U(c) + 1.5Cl_2(g) = UCl_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	24.500	38.000	38.000	0	-206.000	-189.919	139.213
300	24.500	38.150	38.000	.045	-205.990	-189.819	138.281
400	24.680	45.210	38.960	2.500	-205.465	-184.511	100.811
500	25.160	50.770	40.790	4.990	-204.991	-179.329	78.384
600	25.770	55.410	42.852	7.535	-204.546	-174.240	63.466
700	26.420	59.430	44.937	10.145	-204.121	-169.221	52.832
800	27.110	63.000	46.969	12.825	-203.724	-164.259	44.873
900	27.820	66.240	48.940	15.570	-203.363	-159.353	38.696
942	28.122	67.516	49.740	16.745	-203.223	-157.303	36.495
942	28.122	67.516	49.740	16.745	-203.890	-157.303	36.495
1000	28.540	69.200	50.815	18.385	-203.624	-154.438	33.752

Phase changes: 942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 20.980 + 7.440\times10^{-3}T + 1.160\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 20.980\times10^{-3}T + 3.720\times10^{-6}T^2 - 1.160\times10^{2}T^{-1} - 6.197$

Formation equations (kcal/mol):

298.15-942 K: $\Delta Hf^\circ = -206.885 + 4.629\times10^{-3}T - 0.634\times10^{-6}T^2 - 130.950T^{-1}$

$\Delta Gf^\circ = -206.885 - 4.629\times10^{-3}T\ln T + 0.634\times10^{-6}T^2 - 65.475T^{-1} + 83.827\times10^{-3}T$

942-1000 K: $\Delta Hf^\circ = -204.475 - 2.516\times10^{-3}T + 3.588\times10^{-6}T^2 - 218.450T^{-1}$

$\Delta Gf^\circ = -204.475 + 2.516\times10^{-3}T\ln T - 3.588\times10^{-6}T^2 - 109.225T^{-1} + 36.366\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Cordfunke (38). Other data from Parker (186).

$UCl_4(c,l)$
Uranium Tetrachloride
[Formation: $U(c) + 2Cl_2(g) = UCl_4(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15	29.100	47.140	47.140	0	-243.600	-222.300	162.948
300	29.119	47.320	47.140	.054	-243.588	-222.168	161.847
400	30.129	55.836	48.296	3.016	-242.972	-215.123	117.536
500	31.106	62.664	50.508	6.078	-242.352	-208.230	91.016
600	32.068	68.421	53.026	9.237	-241.728	-201.464	73.382
700	33.021	73.435	55.589	12.492	-241.097	-194.802	60.819
800	33.971	77.907	58.106	15.841	-240.473	-188.235	51.423
863	34.568	80.504	59.646	18.000	-240.083	-184.134	46.630
863	38.218	93.134	59.646	28.900	-229.183	-184.134	46.630
900	38.755	94.750	61.057	30.324	-228.819	-182.210	44.246
942	39.364	96.532	62.599	31.964	-228.402	-180.045	41.771
942	39.364	96.532	62.599	31.964	-229.069	-180.045	41.771
1000	40.205	98.908	64.636	34.272	-228.394	-177.048	38.693

Phase changes: 863 K, melting point of UCl_4; $\Delta H°$ = 10.900 kcal/mol.
942 K, α - β transition point of U; $\Delta H°$ = 0.667 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-863 K: $Cp° = 26.430 + 9.454\times10^{-3}T - 0.132\times10^{5}T^{-2}$
$H°-H°_{298} = 26.430\times10^{-3}T + 4.727\times10^{-6}T^{2} + 0.132\times10^{2}T^{-1} - 8.345$
863-1000 K: $Cp° = 25.800 + 14.400\times10^{-3}T$
$H°-H°_{298} = 25.800\times10^{-3}T + 7.200\times10^{-6}T^{2} + 1.272$

Formation equations (kcal/mol):
298.15-863 K: $\Delta Hf° = -245.198 + 5.666\times10^{-3}T + 0.329\times10^{-6}T^{2} - 35.900T^{-1}$
$\Delta Gf° = -245.198 - 5.666\times10^{-3}T\ln T - 0.329\times10^{-6}T^{2} - 17.950T^{-1} + 109.383\times10^{-3}T$
863-942 K: $\Delta Hf° = -235.581 + 5.036\times10^{-3}T + 2.802\times10^{-6}T^{2} - 49.100T^{-1}$
$\Delta Gf° = -235.581 - 5.036\times10^{-3}T\ln T - 2.802\times10^{-6}T^{2} - 24.550T^{-1} + 96.123\times10^{-3}T$
942-1000 K: $\Delta Hf° = -233.171 - 2.109\times10^{-3}T + 7.024\times10^{-6}T^{2} - 136.600T^{-1}$
$\Delta Gf° = -233.171 + 2.109\times10^{-3}T\ln T - 7.024\times10^{-6}T^{2} - 68.300T^{-1} + 48.662\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data from Parker (186).

$UF_3(c)$

Uranium Trifluoride

[Formation: $U(c) + 1.5F_2(g) = UF_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	22.730	29.500	29.500	0	-360.600	-344.153	252.267
300	22.740	29.641	29.501	.042	-360.591	-344.051	250.638
400	23.470	36.282	30.400	2.353	-360.120	-338.609	185.005
500	24.200	41.598	32.126	4.736	-359.679	-333.283	145.676
600	24.930	46.075	34.087	7.193	-359.264	-328.043	119.488
700	25.660	49.973	36.084	9.722	-358.875	-322.871	100.803
800	26.390	53.447	38.041	12.325	-358.517	-317.753	86.805
900	27.120	56.597	39.930	15.000	-358.198	-312.676	75.927
942	27.427	57.841	40.701	16.145	-358.078	-310.555	72.050
942	27.427	57.841	40.701	16.145	-358.745	-310.555	72.050
1000	27.850	59.492	41.743	17.749	-358.504	-307.596	67.224

*Data except enthalpy of formation at 298 K estimated.

Phase change: 942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 20.550 + 7.300\times10^{-3}T$

$H^\circ - H^\circ_{298} = 20.550\times10^{-3}T + 3.650\times10^{-6}T^2 - 6.451$

Formation equations (kcal/mol):

298.15-942 K: $\Delta Hf^\circ = -361.709 + 4.678\times10^{-3}T - 0.833\times10^{-6}T^2 - 63.250T^{-1}$

$\Delta Gf^\circ = -361.709 - 4.678\times10^{-3}T\ln T + 0.833\times10^{-6}T^2 - 31.625T^{-1} + 85.643\times10^{-3}T$

942-1000 K: $\Delta Hf^\circ = -359.299 - 2.467\times10^{-3}T + 3.389\times10^{-6}T^2 - 150.750T^{-1}$

$\Delta Gf^\circ = -359.299 + 2.467\times10^{-3}T\ln T - 3.389\times10^{-6}T^2 - 75.375T^{-1} + 38.182\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data are estimates from Parker (186).

UF_4 (c,1)
Uranium Tetrafluoride
[Formation: $U(c) + 2F_2(g) = UF_4(c,1)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	27.730	36.250	36.250	0	-459.100	-437.444	320.651
300	27.765	36.422	36.252	.051	-459.089	-437.310	318.576
400	29.066	44.608	37.358	2.900	-458.464	-430.144	235.017
500	29.795	51.179	39.487	5.846	-457.862	-423.133	184.949
600	30.296	56.658	41.905	8.852	-457.313	-416.241	151.614
700	30.690	61.359	44.356	11.902	-456.827	-409.434	127.829
800	31.026	65.479	46.744	14.988	-456.418	-402.695	110.010
900	31.328	69.151	49.033	18.106	-456.091	-395.997	96.160
942	31.446	70.583	49.962	19.424	-455.983	-393.196	91.223
942	31.446	70.583	49.962	19.424	-456.650	-393.196	91.223
1000	31.610	72.466	51.213	21.253	-456.439	-389.297	85.080
1049	31.741	73.981	52.241	22.805	-456.256	-386.011	80.421
1049	31.741	73.981	52.241	22.805	-457.393	-386.011	80.421
1100	31.878	75.492	53.286	24.427	-457.143	-382.547	76.004
1200	32.137	78.277	55.254	27.628	-456.639	-375.788	68.439
1300	32.390	80.859	57.124	30.855	-456.117	-369.069	62.045
1309	32.412	81.083	57.288	31.147	-456.069	-368.467	61.518
1309	39.570	89.662	57.288	42.377	-444.839	-368.467	61.518
1400	39.570	92.322	59.481	45.978	-443.709	-363.198	56.697

Phase changes: 942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1309 K, melting point of UF_4; ΔH° = 11.230 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1309 K: $Cp^\circ = 29.531 + 2.300\times10^{-3}T - 2.210\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 29.531\times10^{-3}T + 1.150\times10^{-6}T^2 + 2.210\times10^{2}T^{-1} - 9.648$

1309-1400 K: $Cp^\circ = 39.570$

$H^\circ - H^\circ_{298} = 39.570\times10^{-3}T - 9.420$

Formation equations (kcal/mol):

298.15-942 K: $\Delta Hf^\circ = -461.961 + 9.405\times10^{-3}T - 3.420\times10^{-6}T^2 + 107.500T^{-1}$

$\Delta Gf^\circ = -461.961 - 9.405\times10^{-3}T\ln T + 3.420\times10^{-6}T^2 + 53.750T^{-1} + 134.192\times10^{-3}T$

942-1049 K: $\Delta Hf^\circ = -459.551 + 2.260\times10^{-3}T + 0.802\times10^{-6}T^2 + 20.000T^{-1}$

$\Delta Gf^\circ = -459.551 - 2.260\times10^{-3}T\ln T - 0.802\times10^{-6}T^2 + 10.000T^{-1} + 86.731\times10^{-3}T$

1049-1309 K: $\Delta Hf^\circ = -461.847 + 3.365\times10^{-3}T + 0.802\times10^{-6}T^2 + 20.000T^{-1}$

$\Delta Gf^\circ = -461.847 - 3.365\times10^{-3}T\ln T - 0.802\times10^{-6}T^2 + 10.000T^{-1} + 96.606\times10^{-3}T$

1309-1400 K: $\Delta Hf^\circ = -461.618 + 13.404\times10^{-3}T - 0.348\times10^{-6}T^2 - 201.000T^{-1}$

$\Delta Gf^\circ = -461.618 - 13.404\times10^{-3}T\ln T + 0.348\times10^{-6}T^2 - 100.500T^{-1} + 167.041\times10^{-3}T$

Source: Data from Parker (186).

$UF_4(g)$

Uranium Tetrafluoride (ideal gas)

[Formation: $U(c,l) + 2F_2(g) = UF_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	21.815	88.376	88.376	0	-383.700	-377.585	276.774
300	21.852	88.511	88.378	.040	-383.700	-377.548	275.040
400	23.304	95.018	89.253	2.306	-383.658	-375.502	205.162
500	24.114	100.313	90.973	4.670	-383.638	-373.477	163.244
600	24.598	104.756	92.893	7.118	-383.647	-371.434	135.293
700	24.906	108.573	94.867	9.594	-383.735	-369.392	115.328
800	25.114	111.913	96.793	12.096	-383.910	-367.334	100.350
900	25.259	114.880	98.641	14.615	-384.182	-365.244	88.692
942	25.304	116.033	99.391	15.677	-384.330	-364.358	84.532
942	25.304	116.033	99.391	15.677	-384.997	-364.358	84.532
1000	25.365	117.547	100.401	17.146	-385.146	-363.085	79.351
1049	25.404	118.761	101.230	18.390	-385.271	-362.000	75.419
1049	25.404	118.761	101.230	18.390	-386.408	-362.000	75.419
1100	25.444	119.968	102.071	19.687	-386.483	-360.810	71.685
1200	25.505	122.185	103.657	22.234	-386.633	-358.471	65.286
1300	25.553	124.228	105.161	24.787	-386.785	-356.117	59.868
1400	25.591	126.123	106.591	27.345	-386.942	-353.752	55.222
1408	25.593	126.269	106.702	27.550	-386.954	-353.562	54.879
1408	25.593	126.269	106.702	27.550	-389.139	-353.562	54.879
1500	25.622	127.890	107.953	29.905	-389.516	-351.227	51.173

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 942 K, α - β transition point of U; ΔH° = 0.667 kcal/mol.
1049 K, β - γ transition point of U; ΔH° = 1.137 kcal/mol.
1408 K, melting point of U; ΔH° = 2.185 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp^\circ = 24.982 + 0.648\times10^{-3}T - 2.987\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 24.982\times10^{-3}T + 0.324\times10^{-6}T^2 + 2.987\times10^{2}T^{-1} - 8.479$

Formation equations (kcal/mol):

298.15-942 K: $\Delta Hf^\circ = -385.392 + 4.856\times10^{-3}T - 4.246\times10^{-6}T^2 + 185.200T^{-1}$

$\Delta Gf^\circ = -385.392 - 4.856\times10^{-3}T\ln T + 4.246\times10^{-6}T^2 + 92.600T^{-1} + 51.543\times10^{-3}T$

942-1049 K: $\Delta Hf^\circ = -382.982 - 2.289\times10^{-3}T - 0.024\times10^{-6}T^2 + 97.700T^{-1}$

$\Delta Gf^\circ = -382.982 + 2.289\times10^{-3}T\ln T + 0.024\times10^{-6}T^2 + 48.850T^{-1} + 4.082\times10^{-3}T$

1049-1408 K: $\Delta Hf^\circ = -385.278 - 1.184\times10^{-3}T - 0.024\times10^{-6}T^2 + 97.700T^{-1}$

$\Delta Gf^\circ = -385.278 + 1.184\times10^{-3}T\ln T + 0.024\times10^{-6}T^2 + 48.850T^{-1} + 13.957\times10^{-3}T$

1408-1500 K: $\Delta Hf^\circ = -383.971 - 3.664\times10^{-3}T - 0.024\times10^{-6}T^2 + 97.700T^{-1}$

$\Delta Gf^\circ = -383.971 + 3.664\times10^{-3}T\ln T + 0.024\times10^{-6}T^2 + 48.850T^{-1} - 4.951\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data are estimates from Parker (186).

$UF_5(g)$

Uranium Pentafluoride (ideal gas)

[Formation: $U(c,l) + 2.5F_2(g) = UF_5(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	26.222	93.055	93.055	0	-464.000	-452.058	331.363
300	26.270	93.218	93.055	.049	-463.998	-451.984	329.266
400	28.222	101.069	94.112	2.783	-463.872	-447.996	244.771
500	29.342	107.498	96.166	5.666	-463.736	-444.043	194.089
600	30.022	112.913	98.520	8.636	-463.638	-440.117	160.311
700	30.460	117.576	100.916	11.662	-463.600	-436.199	136.186
800	30.756	121.664	103.259	14.724	-463.646	-432.286	118.093
900	30.965	125.298	105.509	17.810	-463.786	-428.354	104.017
942	31.029	126.712	106.423	19.112	-463.878	-426.699	98.996
942	31.029	126.712	106.423	19.112	-464.545	-426.699	98.996
1000	31.117	128.570	107.655	20.915	-464.616	-424.370	92.745
1049	31.173	130.060	108.667	22.441	-464.675	-422.396	88.001
1049	31.173	130.060	108.667	22.441	-465.812	-422.396	88.001
1100	31.231	131.541	109.694	24.032	-465.820	-420.284	83.502
1200	31.319	134.262	111.629	27.160	-465.835	-416.144	75.789
1300	31.388	136.772	113.468	30.295	-465.852	-412.002	69.263
1400	31.443	139.100	115.216	33.437	-465.875	-407.860	63.669
1408	31.447	139.279	115.353	33.689	-465.877	-407.529	63.256
1408	31.447	139.279	115.353	33.689	-468.062	-407.529	63.256
1500	31.487	141.271	116.882	36.584	-468.314	-403.565	58.799

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 942 K, α - β transition point of U; $\Delta H°$ = 0.667 kcal/mol.
1049 K, β - γ transition point of U; $\Delta H°$ = 1.137 kcal/mol.
1408 K, melting point of U; $\Delta H°$ = 2.185 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp° = 30.562 + 0.902\times10^{-3}T - 4.097\times10^{5}T^{-2}$

$H°- H°_{298} = 30.562\times10^{-3}T + 0.451\times10^{-6}T^2 + 4.097\times10^{2}T^{-1} - 10.526$

Formation equations (kcal/mol):

298.15-942 K: $\Delta Hf° = -466.294 + 6.182\times10^{-3}T - 4.206\times10^{-6}T^2 + 245.950T^{-1}$

$\Delta Gf° = -466.294 - 6.182\times10^{-3}T\ln T + 4.206\times10^{-6}T^2 + 122.975T^{-1} + 80.332\times10^{-3}T$

942-1049 K: $\Delta Hf° = -463.884 - 0.963\times10^{-3}T + 0.016\times10^{-6}T^2 + 158.450T^{-1}$

$\Delta Gf° = -463.884 + 0.963\times10^{-3}T\ln T - 0.016\times10^{-6}T^2 + 79.225T^{-1} + 32.871\times10^{-3}T$

1049-1408 K: $\Delta Hf° = -466.180 + 0.142\times10^{-3}T + 0.016\times10^{-6}T^2 + 158.450T^{-1}$

$\Delta Gf° = -466.180 - 0.142\times10^{-3}T\ln T - 0.016\times10^{-6}T^2 + 79.225T^{-1} + 42.746\times10^{-3}T$

1408-1500 K: $\Delta Hf° = -464.873 - 2.338\times10^{-3}T + 0.016\times10^{-6}T^2 + 158.450T^{-1}$

$\Delta Gf° = -464.873 + 2.338\times10^{-3}T\ln T - 0.016\times10^{-6}T^2 + 79.225T^{-1} + 23.838\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data are estimates from Parker (186).

$UF_6(g)$

Uranium Hexafluoride (ideal gas)

[Formation: $U(c,l) + 3F_2(g) = UF_6(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	30.985	90.233	90.233	0	-513.250	-493.245	361.554
300	31.044	90.425	90.235	.057	-513.247	-493.122	359.235
400	33.436	99.717	91.485	3.293	-513.004	-486.447	265.779
500	34.797	107.337	93.915	6.711	-512.734	-479.838	209.734
600	35.620	113.760	96.702	10.235	-512.497	-473.283	172.391
700	36.149	119.293	99.543	13.825	-512.319	-466.762	145.728
800	36.506	124.145	102.321	17.459	-512.224	-460.264	125.737
900	36.757	128.460	104.990	21.123	-512.222	-453.766	110.188
942	36.834	130.138	106.074	22.668	-512.255	-451.038	104.642
942	36.834	130.138	106.074	22.668	-512.922	-451.038	104.642
1000	36.941	132.343	107.535	24.808	-512.912	-447.232	97.741
1049	37.008	134.112	108.735	26.620	-512.902	-444.013	92.505
1049	37.008	134.112	108.735	26.620	-514.039	-444.013	92.505
1100	37.078	135.871	109.954	28.509	-513.975	-440.609	87.540
1200	37.184	139.102	112.250	32.223	-513.849	-433.946	79.031
1300	37.267	142.081	114.431	35.945	-513.727	-427.290	71.833
1400	37.333	144.846	116.506	39.676	-513.611	-420.648	65.665
1408	37.337	145.059	116.668	39.975	-513.602	-420.117	65.210
1408	37.337	145.059	116.668	39.975	-515.787	-420.117	65.210
1500	37.387	147.423	118.482	43.412	-515.912	-413.861	60.299
1600	37.431	149.838	120.367	47.153	-516.052	-407.054	55.600
1700	37.468	152.108	122.168	50.898	-516.194	-400.234	51.453
1800	37.499	154.251	123.892	54.646	-516.345	-393.410	47.766
1900	37.525	156.279	125.544	58.397	-516.496	-386.574	44.466
2000	37.547	158.204	127.128	62.151	-516.656	-379.734	41.495

Phase changes: 942 K, α - β transition point of U; $\Delta H° = 0.667$ kcal/mol.
1049 K, β - γ transition point of U; $\Delta H° = 1.137$ kcal/mol.
1408 K, melting point of U; $\Delta H° = 2.185$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 36.595 + 0.720\times10^{-3}T - 5.178\times10^{5}T^{-2}$

$H°- H°_{298} = 36.595\times10^{-3}T + 0.360\times10^{-6}T^{2} + 5.178\times10^{2}T^{-1} - 12.680$

Formation equations (kcal/mol):

298.15-942 K: $\Delta Hf° = -516.253 + 7.961\times10^{-3}T - 4.384\times10^{-6}T^{2} + 303.800T^{-1}$

$\Delta Gf° = -516.253 - 7.961\times10^{-3}T\ln T + 4.384\times10^{-6}T^{2} + 151.900T^{-1} + 119.510\times10^{-3}T$

942-1049 K: $\Delta Hf° = -513.843 + 0.816\times10^{-3}T - 0.162\times10^{-6}T^{2} + 216.300T^{-1}$

$\Delta Gf° = -513.843 - 0.816\times10^{-3}T\ln T + 0.162\times10^{-6}T^{2} + 108.150T^{-1} + 72.049\times10^{-3}T$

1049-1408 K: $\Delta Hf° = -516.139 + 1.921\times10^{-3}T - 0.162\times10^{-6}T^{2} + 216.300T^{-1}$

$\Delta Gf° = -516.139 - 1.921\times10^{-3}T\ln T + 0.162\times10^{-6}T^{2} + 108.150T^{-1} + 81.924\times10^{-3}T$

1408-2000 K: $\Delta Hf° = -514.832 - 0.559\times10^{-3}T - 0.162\times10^{-6}T^{2} + 216.300T^{-1}$

$\Delta Gf° = -514.832 + 0.559\times10^{-3}T\ln T + 0.162\times10^{-6}T^{2} + 108.150T^{-1} + 63.016\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data from Parker (186).

$UI_3(c)$
Uranium Triiodide
[Formation: $U(c) + 1.5I_2(c,l,g) = UI_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	26.830	53.000	53.000	0	-110.100	-109.910	80.565
300	26.840	53.170	53.003	.050	-110.098	-109.909	80.068
386.8	27.343	60.051	53.842	2.402	-110.151	-109.854	62.069
386.8	27.343	60.051	53.842	2.402	-115.715	-109.854	62.069
400	27.420	60.970	54.063	2.763	-115.829	-109.652	59.910
458.4	27.759	64.728	55.186	4.374	-116.328	-108.711	51.829
458.4	27.759	64.728	55.186	4.374	-131.359	-108.711	51.829
500	28.000	67.150	56.082	5.534	-131.071	-106.666	46.623
600	28.580	72.300	58.362	8.363	-130.385	-101.848	37.097
700	29.160	76.750	60.679	11.250	-129.714	-97.144	30.329
800	29.740	80.680	62.936	14.195	-129.074	-92.534	25.279

*Data except enthalpy of formation and entropy at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp^\circ = 25.116 + 5.778\times10^{-3}T - 0.007\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.116\times10^{-3}T + 2.889\times10^{-6}T^2 + 0.007\times10^{2}T^{-1} - 7.747$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -110.881 + 2.690\times10^{-3}T - 3.571\times10^{-6}T^2 + 88.200T^{-1}$

$\Delta Gf^\circ = -110.881 - 2.690\times10^{-3}T\ln T + 3.571\times10^{-6}T^2 + 44.100T^{-1} + 17.024\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -113.063 - 6.916\times10^{-3}T - 1.333\times10^{-6}T^2 + 88.200T^{-1}$

$\Delta Gf^\circ = -113.063 + 6.916\times10^{-3}T\ln T + 1.333\times10^{-6}T^2 + 44.100T^{-1} - 33.699\times10^{-3}T$

458.4-800 K: $\Delta Hf^\circ = -135.133 + 8.594\times10^{-3}T - 1.435\times10^{-6}T^2 + 65.250T^{-1}$

$\Delta Gf^\circ = -135.133 - 8.594\times10^{-3}T\ln T + 1.435\times10^{-6}T^2 + 32.625T^{-1} + 109.495\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data from Parker (186), who estimated all except entropy at 298 K.

$UI_4(c,l)$
Uranium Tetraiodide
[Formation: $U(c) + 2I_2(c,l,g) = UI_4(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	30.200	63.000	63.000	0	-122.400	-121.054	88.734
300	30.270	63.190	63.003	.056	-122.404	-121.045	88.180
386.8	32.466	71.195	63.968	2.795	-122.674	-120.621	68.152
386.8	32.466	71.195	63.968	2.795	-130.092	-120.621	68.152
400	32.800	72.290	64.225	3.226	-130.264	-120.295	65.725
458.4	33.559	76.821	65.544	5.170	-130.993	-118.782	56.631
458.4	33.559	76.821	65.544	5.170	-151.035	-118.782	56.631
500	34.100	79.760	66.606	6.577	-150.685	-115.867	50.645
600	34.920	86.060	69.342	10.031	-149.822	-108.989	39.699
700	35.500	91.480	72.119	13.553	-148.966	-102.245	31.922
779	35.880	95.300	74.282	16.373	-148.314	-97.009	27.216
779	39.600	107.110	74.282	25.573	-139.114	-97.009	27.216
800	39.600	108.160	75.155	26.404	-138.870	-95.876	26.192

*Entropy and heat capacity at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
779 K, melting point of UI_4; ΔH° = 9.200 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-779 K: $Cp^\circ = 34.816 + 2.358\times10^{-3}T - 4.728\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 34.816\times10^{-3}T + 1.179\times10^{-6}T^2 + 4.728\times10^{2}T^{-1} - 12.071$

779-800 K: $Cp^\circ = 39.600$
$H^\circ - H^\circ_{298} = 39.600\times10^{-3}T - 5.275$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -125.518 + 5.952\times10^{-3}T - 6.027\times10^{-6}T^2 + 560.300T^{-1}$
$\Delta Gf^\circ = -125.518 - 5.952\times10^{-3}T\ln T + 6.027\times10^{-6}T^2 + 280.150T^{-1} + 43.938\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -128.428 - 6.856\times10^{-3}T - 3.043\times10^{-6}T^2 + 560.300T^{-1}$
$\Delta Gf^\circ = -128.428 + 6.856\times10^{-3}T\ln T + 3.043\times10^{-6}T^2 + 280.150T^{-1} - 23.693\times10^{-3}T$

458.4-779 K: $\Delta Hf^\circ = -157.855 + 13.824\times10^{-3}T - 3.179\times10^{-6}T^2 + 529.700T^{-1}$
$\Delta Gf^\circ = -157.855 - 13.824\times10^{-3}T\ln T + 3.179\times10^{-6}T^2 + 264.850T^{-1} + 167.233\times10^{-3}T$

779-800 K: $\Delta Hf^\circ = -151.059 + 18.608\times10^{-3}T - 4.358\times10^{-6}T^2 + 56.900T^{-1}$
$\Delta Gf^\circ = -151.059 - 18.608\times10^{-3}T\ln T + 4.358\times10^{-6}T^2 + 28.450T^{-1} + 189.832\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (255). Other data from Parker (186) who estimated entropy and heat capacity at 298 K.

$VCl_2(c)$
Vanadium Dichloride
[Formation: $V(c) + Cl_2(g) = VCl_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	17.176	23.200	23.200	0	-108.000	-96.967	71.078
300	17.192	23.306	23.200	.032	-107.994	-96.898	70.589
400	17.848	28.350	23.885	1.786	-107.683	-93.248	50.948
500	18.306	32.384	25.194	3.595	-107.363	-89.675	39.196
600	18.684	35.755	26.680	5.445	-107.032	-86.167	31.386
700	19.026	38.662	28.189	7.331	-106.688	-82.718	25.825
800	19.348	41.223	29.660	9.250	-106.332	-79.318	21.668
900	19.658	43.520	31.076	11.200	-105.965	-75.962	18.446
1000	19.962	45.607	32.426	13.181	-105.589	-72.650	15.877
1100	20.260	47.524	33.713	15.192	-105.203	-69.375	13.783
1200	20.556	49.299	34.938	17.233	-104.811	-66.134	12.044
1300	20.849	50.956	36.108	19.303	-104.414	-62.927	10.579

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $Cp^\circ = 17.186 + 2.852\times10^{-3}T - 0.764\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 17.186\times10^{-3}T + 1.426\times10^{-6}T^2 + 0.764\times10^{2}T^{-1} - 5.507$

Formation equations (kcal/mol):

298.15-1300 K: $\Delta Hf^\circ = -109.068 + 3.248\times10^{-3}T + 0.226\times10^{-6}T^2 + 23.800T^{-1}$

$\Delta Gf^\circ = -109.068 - 3.248\times10^{-3}T\ln T - 0.226\times10^{-6}T^2 + 11.900T^{-1} + 59.027\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (254). Low-temperature heat capacities and entropy at 298 K from Shomate (213). High-temperature data based on King (125).

$VCl_3(c)$

Vanadium Trichloride

[Formation: $V(c) + 1.5Cl_2(g) = VCl_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	22.270	31.300	31.300	0	-138.890	-122.328	89.668
300	22.304	31.438	31.301	.041	-138.882	-122.225	89.040
400	23.647	38.068	32.195	2.349	-138.432	-116.739	63.783
500	24.370	43.429	33.923	4.753	-137.944	-111.371	48.680
600	24.870	47.919	35.892	7.216	-137.434	-106.104	38.648
700	25.266	51.783	37.893	9.723	-136.909	-100.925	31.510
800	25.605	55.179	39.845	12.267	-136.370	-95.822	26.177
900	25.911	58.213	41.721	14.843	-135.822	-90.784	22.045

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-900 K: $Cp° = 24.223 + 2.170\times10^{-3}T - 2.312\times10^{5}T^{-2}$

$H°- H°_{298} = 24.223\times10^{-3}T + 1.085\times10^{-6}T^{2} + 2.312\times10^{2}T^{-1} - 8.094$

Formation equations (kcal/mol):

298.15-900 K: $\Delta Hf° = -141.111 + 5.872\times10^{-3}T - 0.159\times10^{-6}T^{2} + 144.450T^{-1}$

$\Delta Gf° = -141.111 - 5.872\times10^{-3}T\ln T + 0.159\times10^{-6}T^{2} + 72.225T^{-1} + 95.593\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mrazek (161). Low-temperature heat capacities and entropy at 298 K from Shomate (213). High-temperature data based on King (125).

$VCl_4(g)$
Vanadium Tetrachloride (ideal gas)
[Formation: $V(c) + 2Cl_2(g) = VCl_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	22.960	87.580	87.580	0	-125.600	-117.873	86.402
300	22.990	87.720	87.580	.050	-125.591	-117.817	85.829
400	24.080	94.500	88.475	2.410	-125.504	-115.239	62.963
500	24.660	99.940	90.240	4.850	-125.406	-112.681	49.252
600	25.000	104.470	92.253	7.330	-125.314	-110.150	40.122
700	25.210	108.340	94.283	9.840	-125.224	-107.632	33.604
800	25.350	111.720	96.257	12.370	-125.143	-105.128	28.719
900	25.450	114.710	98.143	14.910	-125.076	-102.626	24.921
1000	25.520	117.390	99.930	17.460	-125.025	-100.131	21.883
1100	25.580	119.830	101.639	20.010	-124.997	-97.653	19.402
1200	25.620	122.060	103.252	22.570	-124.986	-95.171	17.333
1300	25.650	124.110	104.772	25.140	-124.991	-92.677	15.580
1400	25.670	126.010	106.224	27.700	-125.034	-90.194	14.080
1500	25.690	127.780	107.600	30.270	-125.096	-87.698	12.777

Phase changes: 247 K, melting point of VCl_4; ΔH° = 0.550 kcal/mol.
428 K, boiling point of VCl_4; ΔH° = 9.5 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp^\circ = 26.547 - 0.630\times10^{-3}T - 3.644\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 26.547\times10^{-3}T - 0.315\times10^{-6}T^2 + 3.644\times10^{2}T^{-1} - 9.109$

Formation equations (kcal/mol):

298.15-1500 K: $\Delta Hf^\circ = -127.402 + 3.782\times10^{-3}T - 1.603\times10^{-6}T^2 + 243.500T^{-1}$

$\Delta Gf^\circ = -127.402 - 3.782\times10^{-3}T\ln T + 1.603\times10^{-6}T^2 + 121.750T^{-1} + 51.659\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (254). Fusion data from Whittaker (264). Boiling data from Tret'yakova (245). Other data based on Creighton (40) and Clark (30).

$VF_3(c)$

Vanadium Trifluoride

[Formation: $V(c) + 1.5F_2(g) = VF_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	21.500	23.200	23.200	0	-310.000	-293.190	214.912
300	21.550	23.330	23.200	.040	-309.992	-293.085	213.510
400	23.220	29.790	24.065	2.290	-309.508	-287.519	157.091
500	23.990	35.070	25.760	4.655	-308.986	-282.085	123.298
600	24.400	39.480	27.688	7.075	-308.460	-276.754	100.806
700	24.630	43.260	29.646	9.530	-307.941	-271.509	84.768
800	24.780	46.560	31.560	12.000	-307.441	-266.341	72.760
900	24.860	49.490	33.401	14.480	-306.961	-261.238	63.436
1000	24.920	52.110	35.140	16.970	-306.502	-256.182	55.988

*Data estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 25.537 - 0.264\times10^{-3}T - 3.535\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.537\times10^{-3}T - 0.132\times10^{-6}T^2 + 3.535\times10^{2}T^{-1} - 8.788$

Formation equations (kcal/mol):

298.15-1000 K: $\Delta Hf^\circ = -312.884 + 7.664\times10^{-3}T - 1.505\times10^{-6}T^2 + 218.450T^{-1}$

$\Delta Gf^\circ = -312.884 - 7.664\times10^{-3}T\ln T + 1.505\times10^{-6}T^2 + 109.225T^{-1} + 108.041\times10^{-3}T$

Sources: Enthalpy of formation estimated using Pillai (194). Other data estimated using Myers (168).

VF_5(g)
Vanadium Pentafluoride (ideal gas)
[Formation: $V(c) + 2.5F_2(g) = VF_5(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	23.560	77.860	77.860	0	-343.250	-328.294	240.643
300	23.620	78.000	77.860	.044	-343.252	-328.200	239.090
400	26.300	85.200	78.822	2.551	-343.281	-323.175	176.573
500	27.930	91.260	80.716	5.272	-343.206	-318.154	139.063
600	28.960	96.450	82.922	8.117	-343.086	-313.158	114.066
700	29.640	100.970	85.179	11.054	-342.933	-308.178	96.216
800	30.110	104.960	87.411	14.039	-342.780	-303.229	82.837
900	30.440	108.520	89.558	17.066	-342.623	-298.287	72.433
1000	30.690	111.740	91.613	20.127	-342.473	-293.367	64.115
1100	30.870	114.680	93.582	23.208	-342.335	-288.466	57.312
1200	31.010	117.370	95.451	26.303	-342.216	-283.571	51.645
1300	31.130	119.860	97.244	29.401	-342.127	-278.699	46.853
1400	31.220	122.170	98.939	32.523	-342.050	-273.821	42.745
1500	31.290	124.320	100.559	35.642	-342.009	-268.946	39.185
1600	31.350	126.340	102.106	38.775	-341.986	-264.073	36.070
1700	31.400	128.250	103.595	41.913	-341.988	-259.215	33.324
1800	31.440	130.040	105.004	45.065	-342.014	-254.324	30.879
1900	31.480	131.740	106.368	48.206	-342.085	-249.452	28.693
2000	31.510	133.360	107.687	51.347	-342.198	-244.593	26.728

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 29.866 + 1.156\times10^{-3}T - 5.912\times10^{5}T^{-2}$

$H°- H°_{298} = 29.866\times10^{-3}T + 0.578\times10^{-6}T^{2} + 5.912\times10^{2}T^{-1} - 10.939$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -345.396 + 3.485\times10^{-3}T - 0.969\times10^{-6}T^{2} + 355.650T^{-1}$

$\Delta Gf° = -345.396 - 3.485\times10^{-3}T\ln T + 0.969\times10^{-6}T^{2} + 177.825T^{-1} + 74.926\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Johnson (109). Other data from Vizi (250).

WBr(g)

Tungsten Monobromide (ideal gas)

[Formation: $W(c) + 0.5Br_2(l,g) = WBr(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	8.612	65.130	65.130	0	140.100	128.430	-94.141
300	8.616	65.183	65.130	.016	140.089	128.359	-93.508
332.6	8.665	66.074	65.179	.298	139.886	127.095	-83.512
332.6	8.665	66.074	65.179	.298	136.354	127.095	-83.512
400	8.767	67.685	65.470	.886	136.247	125.228	-68.420
500	8.846	69.651	66.117	1.767	136.081	122.491	-53.540
600	8.895	71.268	66.845	2.654	135.906	119.786	-43.631
700	8.931	72.642	67.576	3.546	135.725	117.118	-36.565
800	8.961	73.837	68.287	4.440	135.540	114.468	-31.271
900	8.992	74.894	68.963	5.338	135.347	111.851	-27.161
1000	9.025	75.843	69.604	6.239	135.153	109.251	-23.876
1100	9.062	76.705	70.211	7.143	134.953	106.679	-21.195
1200	9.102	77.495	70.786	8.051	134.747	104.110	-18.961
1300	9.144	78.225	71.330	8.963	134.538	101.571	-17.075
1400	9.189	78.905	71.848	9.880	134.323	99.053	-15.463
1500	9.234	79.540	72.339	10.801	134.104	96.537	-14.065
1600	9.279	80.137	72.808	11.727	133.881	94.043	-12.845
1700	9.324	80.701	73.256	12.657	133.654	91.567	-11.772
1800	9.369	81.236	73.685	13.592	133.422	89.085	-10.816
1900	9.413	81.743	74.095	14.531	133.187	86.634	-9.965
2000	9.458	82.227	74.490	15.474	132.946	84.183	-9.199

*Data estimated.

Phase change: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.763 + 0.312\times10^{-3}T - 0.217\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.763\times10^{-3}T + 0.156\times10^{-6}T^2 + 0.217\times10^{2}T^{-1} - 2.699$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = 141.930 - 6.098\times10^{-3}T - 0.165\times10^{-6}T^2 + 0.700T^{-1}$

$\Delta Gf^\circ = 141.930 + 6.098\times10^{-3}T\ln T + 0.165\times10^{-6}T^2 + 0.350T^{-1} - 80.074\times10^{-3}T$

332.6-2000 K: $\Delta Hf^\circ = 136.930 - 1.517\times10^{-3}T - 0.242\times10^{-6}T^2 - 15.000T^{-1}$

$\Delta Gf^\circ = 136.930 + 1.517\times10^{-3}T\ln T + 0.242\times10^{-6}T^2 - 7.500T^{-1} - 38.396\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

$WBr_5(c,l,g)$
Tungsten Pentabromide
[Formation: $W(c) + 2.5Br_2(l,g) = WBr_5(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	37.156	65.000	65.000	0	-74.500	-64.438	47.234
300	37.200	65.230	65.000	.069	-74.524	-64.373	46.895
332.6	37.982	69.108	65.216	1.294	-74.959	-63.249	41.560
332.6	37.982	69.108	65.216	1.294	-92.622	-63.249	41.560
400	39.600	76.260	66.488	3.909	-91.881	-57.372	31.346
500	42.000	85.351	69.377	7.987	-90.614	-48.889	21.369
559	43.400	90.120	71.319	10.510	-89.762	-44.016	17.208
559	43.500	97.455	71.319	14.610	-85.662	-44.016	17.208
600	43.500	100.534	73.211	16.394	-85.045	-40.983	14.928
633.5	43.500	102.898	74.720	17.851	-84.543	-38.537	13.295
633.5	31.466	133.657	74.719	37.337	-65.057	-38.537	13.295
700	31.529	136.804	80.474	39.431	-64.866	-35.763	11.166
800	31.591	141.019	87.784	42.588	-64.578	-31.626	8.640
900	31.636	144.742	93.910	45.749	-64.306	-27.520	6.683
1000	31.672	148.077	99.162	48.915	-64.035	-23.447	5.124
1100	31.704	151.097	103.749	52.083	-63.775	-19.392	3.853
1200	31.735	153.857	107.811	55.255	-63.523	-15.375	2.800
1300	31.768	156.399	111.453	58.430	-63.279	-11.369	1.911
1400	31.805	158.754	114.748	61.609	-63.044	-7.372	1.151
1500	31.845	160.950	117.755	64.792	-62.817	-3.410	.497
1600	31.889	163.007	120.521	67.978	-62.599	.546	-.075
1700	31.937	164.941	123.077	71.169	-62.385	4.492	-.577
1800	31.987	166.768	125.454	74.366	-62.176	8.410	-1.021
1900	32.039	168.499	127.674	77.567	-61.973	12.333	-1.419
2000	32.093	170.144	129.757	80.774	-61.778	16.229	-1.773

*Data except enthalpy of formation at 298 K and temperature of fusion estimated.

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
559 K, melting point of WBr_5; $\Delta H°$ = 4.100 kcal/mol.
633.5 K, boiling point of WBr_5; $\Delta H°$ = 19.486 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-559 K: $Cp° = 30.006 + 24.000\times10^{-3}T$
$H°- H°_{298} = 30.006\times10^{-3}T + 12.000\times10^{-6}T^2 - 10.013$

559-633.5 K: $Cp° = 43.501$
$H°- H°_{298} = 43.501\times10^{-3}T - 9.707$

633.5-2000 K: $Cp° = 31.551 + 0.230\times10^{-3}T - 0.924\times10^{5}T^{-2}$
$H°- H°_{298} = 31.551\times10^{-3}T + 0.115\times10^{-6}T^2 + 0.924\times10^{2}T^{-1} + 17.157$

WBr_5(c,l,g) - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -69.213 - 21.037\times10^{-3}T + 11.879\times10^{-6}T^2 - 21.000T^{-1}$

$\Delta Gf^\circ = -69.213 + 21.037\times10^{-3}T\ln T - 11.879\times10^{-6}T^2 - 10.500T^{-1} - 100.181\times10^{-3}T$

332.6-559 K: $\Delta Hf^\circ = -94.214 + 1.866\times10^{-3}T + 11.491\times10^{-6}T^2 - 99.500T^{-1}$

$\Delta Gf^\circ = -94.214 - 1.866\times10^{-3}T\ln T - 11.491\times10^{-6}T^2 - 49.750T^{-1} + 108.207\times10^{-3}T$

559-633.5 K: $\Delta Hf^\circ = -93.908 + 15.361\times10^{-3}T - 0.509\times10^{-6}T^2 - 99.500T^{-1}$

$\Delta Gf^\circ = -93.908 - 15.361\times10^{-3}T\ln T + 0.509\times10^{-6}T^2 - 49.750T^{-1} + 186.322\times10^{-3}T$

633.5-2000 K: $\Delta Hf^\circ = -67.044 + 3.411\times10^{-3}T - 0.394\times10^{-6}T^2 - 7.100T^{-1}$

$\Delta Gf^\circ = -67.044 - 3.411\times10^{-3}T\ln T + 0.394\times10^{-6}T^2 - 3.550T^{-1} + 66.781\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K and temperature of fusion.

$WBr_5(g)$

Tungsten Pentabromide (ideal gas)

[Formation: $W(c) + 2.5Br_2(l,g) = WBr_5(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	30.404	110.252	110.252	0	-47.600	-51.030	37.406
300	30.420	110.441	110.254	.056	-47.637	-51.050	37.189
332.6	30.609	113.589	110.430	1.051	-48.303	-51.387	33.766
332.6	30.609	113.589	110.430	1.051	-65.965	-51.387	33.766
400	31.000	119.282	111.454	3.131	-65.758	-48.458	26.476
500	31.279	126.233	113.739	6.247	-65.453	-44.170	19.306
600	31.434	131.951	116.313	9.383	-65.156	-39.944	14.549
700	31.529	136.804	118.903	12.531	-64.866	-35.763	11.166
800	31.591	141.019	121.409	15.688	-64.578	-31.626	8.640
900	31.636	144.742	123.799	18.849	-64.306	-27.520	6.683
1000	31.672	148.077	126.062	22.015	-64.035	-23.447	5.124
1100	31.704	151.097	128.203	25.183	-63.775	-19.392	3.853
1200	31.735	153.857	130.228	28.355	-63.523	-15.375	2.800
1300	31.768	156.399	132.145	31.530	-63.279	-11.369	1.911
1400	31.805	158.754	133.962	34.709	-63.044	-7.372	1.151
1500	31.845	160.950	135.689	37.892	-62.817	-3.410	.497
1600	31.889	163.007	137.333	41.078	-62.599	.546	-.075
1700	31.937	164.941	138.900	44.269	-62.384	4.492	-.577
1800	31.987	166.768	140.398	47.466	-62.176	8.410	-1.021
1900	32.039	168.499	141.832	50.667	-61.973	12.333	-1.419
2000	32.093	170.144	143.207	53.874	-61.778	16.229	-1.773

*Data except enthalpy of formation at 298 K estimated.

Phase change: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 31.630 + 0.182\times10^{-3}T - 1.139\times10^{5}T^{-2}$

$H°- H°_{298} = 31.630\times10^{-3}T + 0.091\times10^{-6}T^2 + 1.139\times10^{2}T^{-1} - 9.821$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -42.121 - 19.413\times10^{-3}T - 0.030\times10^{-6}T^2 + 92.900T^{-1}$

$\Delta Gf° = -42.121 + 19.413\times10^{-3}T\ln T + 0.030\times10^{-6}T^2 + 46.450T^{-1} - 141.017\times10^{-3}T$

332.6-2000 K: $\Delta Hf° = -67.122 + 3.490\times10^{-3}T - 0.418\times10^{-6}T^2 + 14.400T^{-1}$

$\Delta Gf° = -67.122 - 3.490\times10^{-3}T\ln T + 0.418\times10^{-6}T^2 + 7.200T^{-1} + 67.371\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$WBr_6(c)$

Tungsten Hexabromide

[Formation: $W(c) + 3Br_2(l,g) = WBr_6(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	43.352	75.000	75.000	0	-82.000	-69.496	50.942
300	43.400	75.268	75.001	.080	-82.030	-69.416	50.569
332.60	44.248	79.789	75.253	1.509	-82.555	-68.020	44.695
332.60	44.248	79.789	75.253	1.509	-103.750	-68.020	44.695
400	46.000	88.110	76.735	4.550	-102.877	-60.869	33.257
500	48.600	98.654	80.094	9.280	-101.399	-50.535	22.089
600	51.200	107.744	83.961	14.270	-99.691	-40.520	14.759

*Data except enthalpy of formation at 298 K estimated.

Phase change: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-600 K: $Cp° = 35.600 + 26.000\times10^{-3}T$

$H°- H°_{298} = 35.600\times10^{-3}T + 13.000\times10^{-6}T^2 - 11.770$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -75.778 - 24.488\times10^{-3}T + 12.929\times10^{-6}T^2 - 21.000T^{-1}$

$\Delta Gf° = -75.778 + 24.488\times10^{-3}T\ln T - 12.929\times10^{-6}T^2 - 10.500T^{-1} - 114.482\times10^{-3}T$

332.6-600 K: $\Delta Hf° = -105.779 + 2.995\times10^{-3}T + 12.464\times10^{-6}T^2 - 115.200T^{-1}$

$\Delta Gf° = -105.779 - 2.995\times10^{-3}T\ln T - 12.464\times10^{-6}T^2 - 57.600T^{-1} + 135.583\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$WBr_6(g)$
Tungsten Hexabromide (ideal gas)
[Formation: $W(c) + 3Br_2(l,g) = WBr_6(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	36.178	115.340	115.340	0	-58.100	-57.624	42.239
300	36.196	115.564	115.341	.067	-58.143	-57.618	41.974
332.6	36.412	119.309	115.549	1.251	-58.914	-57.522	37.797
332.6	36.412	119.309	115.549	1.251	-80.109	-57.522	37.797
400	36.858	126.081	116.771	3.724	-79.803	-52.983	28.948
500	37.175	134.343	119.487	7.428	-79.351	-46.331	20.251
600	37.351	141.138	122.546	11.155	-78.906	-39.772	14.487
700	37.457	146.904	125.625	14.895	-78.471	-33.282	10.391
800	37.527	151.911	128.605	18.645	-78.038	-26.856	7.337
900	37.575	156.334	131.445	22.400	-77.621	-20.482	4.974
1000	37.609	160.295	134.136	26.159	-77.207	-14.156	3.094
1100	37.634	163.880	136.678	29.922	-76.803	-7.859	1.562
1200	37.654	167.156	139.084	33.686	-76.410	-1.616	.294
1300	37.669	170.170	141.361	37.452	-76.028	4.606	-.774
1400	37.681	172.962	143.519	41.220	-75.657	10.807	-1.687
1500	37.691	175.562	145.570	44.988	-75.299	16.963	-2.471
1600	37.698	177.995	147.521	48.758	-74.951	23.107	-3.156
1700	37.705	180.281	149.382	52.528	-74.613	29.228	-3.757
1800	37.711	182.436	151.159	56.299	-74.286	35.318	-4.288
1900	37.715	184.475	152.859	60.070	-73.969	41.407	-4.763
2000	37.719	186.410	154.489	63.842	-73.666	47.460	-5.186

*Data estimated.

Phase change: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 37.713 + 0.028\times10^{-3}T - 1.372\times10^{5}T^{-2}$

$H°- H°_{298} = 37.713\times10^{-3}T + 0.014\times10^{-6}T^2 + 1.372\times10^{2}T^{-1} - 11.706$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -51.814 - 22.375\times10^{-3}T - 0.057\times10^{-6}T^2 + 116.200T^{-1}$

$\Delta Gf° = -51.814 + 22.375\times10^{-3}T\ln T + 0.057\times10^{-6}T^2 + 58.100T^{-1} - 147.642\times10^{-3}T$

332.6-2000 K: $\Delta Hf° = -81.815 + 5.108\times10^{-3}T - 0.522\times10^{-6}T^2 + 22.000T^{-1}$

$\Delta Gf° = -81.815 - 5.108\times10^{-3}T\ln T + 0.522\times10^{-6}T^2 + 11.000T^{-1} + 102.423\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

WCl(g)

Tungsten Monochloride (ideal gas)

[Formation: $W(c) + 0.5Cl_2(g) = WCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	8.327	62.567	62.567	0	132.300	123.915	-90.831
300	8.334	62.619	62.569	.015	132.297	123.864	-90.234
400	8.582	65.054	62.896	.863	132.139	121.078	-66.153
500	8.718	66.985	63.529	1.728	131.971	118.331	-51.722
600	8.802	68.583	64.243	2.604	131.795	115.615	-42.112
700	8.859	69.944	64.961	3.488	131.614	112.937	-35.260
800	8.904	71.130	65.660	4.376	131.427	110.278	-30.126
900	8.945	72.181	66.328	5.268	131.233	107.650	-26.141
1000	8.985	73.126	66.961	6.165	131.037	105.040	-22.956
1100	9.027	73.984	67.561	7.065	130.836	102.459	-20.356
1200	9.071	74.771	68.129	7.970	130.629	99.881	-18.191
1300	9.117	75.499	68.668	8.880	130.419	97.334	-16.363
1400	9.164	76.177	69.181	9.794	130.202	94.806	-14.800
1500	9.211	76.810	69.668	10.713	129.982	92.282	-13.445
1600	9.257	77.406	70.133	11.636	129.756	89.778	-12.263
1700	9.303	77.969	70.578	12.564	129.527	87.294	-11.222
1800	9.349	78.502	71.004	13.497	129.294	84.804	-10.297
1900	9.394	79.009	71.412	14.434	129.057	82.343	-9.471
2000	9.439	79.492	71.804	15.375	128.814	79.884	-8.729

*Data estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.704 + 0.348\times10^{-3}T - 0.427\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.704\times10^{-3}T + 0.174\times10^{-6}T^2 + 0.427\times10^{2}T^{-1} - 2.754$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = 132.818 - 1.525\times10^{-3}T - 0.241\times10^{-6}T^2 - 12.450T^{-1}$

$\Delta Gf^\circ = 132.818 + 1.525\times10^{-3}T\ln T + 0.241\times10^{-6}T^2 - 6.225T^{-1} - 38.546\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

$WCl_2(c)$
Tungsten Dichloride
[Formation: $W(c) + Cl_2(g) = WCl_2(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	18.600	31.200	31.200	0	-61.500	-52.588	38.548
300	18.610	31.315	31.202	.034	-61.492	-52.533	38.269
400	19.133	36.740	31.935	1.922	-61.025	-49.615	27.108
500	19.656	41.065	33.343	3.861	-60.545	-46.818	20.464
600	20.179	44.696	34.941	5.853	-60.040	-44.124	16.072
700	20.702	47.845	36.564	7.897	-59.500	-41.509	12.960
800	21.225	50.644	38.153	9.993	-58.922	-38.983	10.649
900	21.750	53.174	39.683	12.142	-58.304	-36.521	8.868

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-900 K: $Cp^\circ = 17.040 + 5.232\times10^{-3}T$

$H^\circ - H^\circ_{298} = 17.040\times10^{-3}T + 2.616\times10^{-6}T^2 - 5.313$

Formation equations (kcal/mol):

298.15-900 K: $\Delta Hf^\circ = -62.107 + 2.398\times10^{-3}T + 2.157\times10^{-6}T^2 - 89.300T^{-1}$

$\Delta Gf^\circ = -62.107 - 2.398\times10^{-3}T\ln T - 2.157\times10^{-6}T^2 - 44.650T^{-1} + 46.735\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$WCl_2(g)$

Tungsten Dichloride (ideal gas)

[Formation: $W(c) + Cl_2(g) = WCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	13.877	73.925	73.925	0	-3.000	-6.827	5.004
300	13.887	74.011	73.925	.026	-3.000	-6.849	4.990
400	14.290	78.068	74.476	1.437	-3.010	-8.131	4.443
500	14.497	81.281	75.527	2.877	-3.029	-9.410	4.113
600	14.617	83.936	76.713	4.334	-3.059	-10.687	3.893
700	14.695	86.195	77.911	5.799	-3.098	-11.952	3.732
800	14.756	88.162	79.072	7.272	-3.143	-13.218	3.611
900	14.814	89.903	80.181	8.750	-3.196	-14.469	3.514
1000	14.881	91.467	81.232	10.235	-3.250	-15.719	3.435
1100	14.960	92.889	82.228	11.727	-3.308	-16.955	3.369
1200	15.056	94.195	83.172	13.228	-3.369	-18.200	3.315
1300	15.168	95.404	84.066	14.739	-3.429	-19.427	3.266
1400	15.295	96.533	84.917	16.262	-3.489	-20.646	3.223
1500	15.434	97.593	85.728	17.798	-3.545	-21.875	3.187
1600	15.582	98.594	86.501	19.349	-3.597	-23.093	3.154
1700	15.735	99.543	87.240	20.915	-3.642	-24.300	3.124
1800	15.890	100.447	87.949	22.496	-3.683	-25.528	3.099
1900	16.043	101.310	88.629	24.093	-3.716	-26.734	3.075
2000	16.192	102.137	89.285	25.705	-3.746	-27.952	3.054

*Data estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 14.315 + 0.736\times10^{-3}T - 0.585\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.315\times10^{-3}T + 0.368\times10^{-6}T^2 + 0.585\times10^{2}T^{-1} - 4.497$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -2.791 - 0.327\times10^{-3}T - 0.091\times10^{-6}T^2 - 30.800T^{-1}$

$\Delta Gf^\circ = -2.791 + 0.327\times10^{-3}T\ln T + 0.091\times10^{-6}T^2 - 15.400T^{-1} - 15.253\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

$WCl_4(c)$

Tungsten Tetrachloride

[Formation: $W(c) + 2Cl_2(g) = WCl_4(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	31.000	47.400	47.400	0	-105.900	-85.930	62.988
300	31.030	47.592	47.402	.057	-105.884	-85.806	62.509
400	32.335	56.697	48.632	3.226	-104.966	-79.249	43.299
500	33.640	64.053	51.005	6.524	-103.980	-72.933	31.878
600	34.945	70.302	53.712	9.954	-102.906	-66.826	24.341
700	36.250	75.786	56.482	13.513	-101.729	-60.901	19.014
800	37.555	80.712	59.207	17.204	-100.442	-55.159	15.068

*Data except enthalpy of formation at 298 K estimated.

Phase change: 770 K, pressure of decomposition products = 1 atm.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-800 K: $Cp^\circ = 27.126 + 13.038\times10^{-3}T - 0.012\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 27.126\times10^{-3}T + 6.519\times10^{-6}T^2 + 0.012\times10^{2}T^{-1} - 8.671$

Formation equations (kcal/mol):

298.15-800 K: $\Delta Hf^\circ = -106.997 + 3.657\times10^{-3}T + 5.972\times10^{-6}T^2 - 156.400T^{-1}$

$\Delta Gf^\circ = -106.997 - 3.657\times10^{-3}T\ln T - 5.972\times10^{-6}T^2 - 78.200T^{-1} + 94.154\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$WCl_4(g)$

Tungsten Tetrachloride (ideal gas)

[Formation: $W(c) + 2Cl_2(g) = WCl_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	23.629	90.624	90.624	0	-80.300	-73.217	53.669
300	23.652	90.770	90.624	.044	-80.297	-73.172	53.305
400	24.526	97.709	91.564	2.458	-80.134	-70.822	38.695
500	24.971	103.235	93.365	4.935	-79.969	-68.513	29.946
600	25.224	107.812	95.402	7.446	-79.814	-66.240	24.127
700	25.381	111.713	97.460	9.977	-79.665	-63.986	19.977
800	25.485	115.110	99.459	12.521	-79.525	-61.760	16.872
900	25.557	118.116	101.368	15.073	-79.394	-59.542	14.459
1000	25.609	120.811	103.180	17.631	-79.269	-57.344	12.532
1100	25.648	123.254	104.896	20.194	-79.153	-55.149	10.957
1200	25.678	125.487	106.520	22.760	-79.049	-52.979	9.649
1300	25.703	127.543	108.058	25.330	-78.952	-50.803	8.541
1400	25.725	129.449	109.520	27.901	-78.868	-48.632	7.592
1500	25.745	131.225	110.908	30.475	-78.792	-46.481	6.772
1600	25.765	132.887	112.231	33.050	-78.728	-44.326	6.055
1700	25.785	134.449	113.492	35.627	-78.671	-42.167	5.421
1800	25.806	135.924	114.698	38.207	-78.624	-40.036	4.861
1900	25.829	137.320	115.852	40.789	-78.584	-37.886	4.358
2000	25.854	138.645	116.959	43.373	-78.557	-35.751	3.907

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 25.656 + 0.120\times10^{-3}T - 1.834\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.656\times10^{-3}T + 0.060\times10^{-6}T^2 + 1.834\times10^{2}T^{-1} - 8.270$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = -80.995 + 2.187\times10^{-3}T - 0.487\times10^{-6}T^2 + 25.800T^{-1}$

$\Delta Gf^\circ = -80.995 - 2.187\times10^{-3}T\ln T + 0.487\times10^{-6}T^2 + 12.900T^{-1} + 38.258\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$WCl_5(c,l,g)$
Tungsten Pentachloride
[Formation: $W(c) + 2.5Cl_2(g) = WCl_5(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	37.200	52.000	52.000	0	-122.600	-96.057	70.411
300	37.255	52.230	52.000	.069	-122.579	-95.891	69.856
400	40.018	63.326	53.493	3.933	-121.382	-87.171	47.627
500	42.781	72.553	56.407	8.073	-119.980	-78.775	34.432
526	43.462	74.739	57.260	9.194	-119.580	-76.643	31.844
526	43.500	84.087	57.260	14.111	-114.663	-76.643	31.844
561.4	43.500	86.920	59.041	15.651	-114.112	-74.106	28.849
561.4	30.812	115.894	59.041	31.917	-97.846	-74.106	28.849
600	30.947	117.951	62.771	33.108	-97.735	-72.481	26.401
700	31.166	122.740	71.004	36.215	-97.450	-68.291	21.321
800	31.311	126.911	77.737	39.339	-97.173	-64.149	17.525
900	31.413	130.605	83.409	42.476	-96.902	-60.031	14.577
1000	31.490	133.919	88.298	45.621	-96.637	-55.951	12.228
1100	31.553	136.924	92.585	48.773	-96.380	-51.887	10.309
1200	31.608	139.671	96.395	51.931	-96.134	-47.859	8.716
1300	31.660	142.204	99.823	55.095	-95.894	-43.841	7.370
1400	31.711	144.552	102.936	58.263	-95.665	-39.836	6.219
1500	31.763	146.741	105.783	61.437	-95.442	-35.860	5.225
1600	31.817	148.793	108.408	64.616	-95.228	-31.893	4.356
1700	31.873	150.723	110.841	67.800	-95.019	-27.929	3.590
1800	31.930	152.547	113.108	70.991	-94.816	-24.003	2.914
1900	31.988	154.275	115.230	74.186	-94.619	-20.068	2.308
2000	32.047	155.917	117.223	77.388	-94.431	-16.155	1.765

*Data except enthalpy of formation at 298 K and temperature and enthalpy of fusion estimated.

Phase changes: 526 K, melting point of WCl_5; $\Delta H°$ = 4.917 kcal/mol.
561.4 K, boiling point of WCl_5; $\Delta H°$ = 16.266 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-526 K: $Cp° = 29.200 + 27.220\times10^{-3}T - 0.103\times10^{5}T^{-2}$
$H°- H°_{298} = 29.200\times10^{-3}T + 13.610\times10^{-6}T^{2} + 0.103\times10^{2}T^{-1} - 9.950$

526-561.4 K: $Cp° = 43.500$
$H°- H°_{298} = 43.500\times10^{-3}T - 8.770$

561.4-2000 K: $Cp° = 31.473 + 0.282\times10^{-3}T - 2.580\times10^{5}T^{-2}$
$H°- H°_{298} = 31.473\times10^{-3}T + 0.141\times10^{-6}T^{2} + 2.580\times10^{2}T^{-1} + 13.744$

Formation equations (kcal/mol):

298.15-526 K: $\Delta Hf° = -123.542 + 1.318\times10^{-3}T + 13.019\times10^{-6}T^{2} - 181.450T^{-1}$
$\Delta Gf° = -123.542 - 1.318\times10^{-3}T\ln T - 13.019\times10^{-6}T^{2} - 90.725T^{-1} + 104.592\times10^{-3}T$

526-561.4 K: $\Delta Hf° = -122.361 + 15.617\times10^{-3}T - 0.591\times10^{-6}T^{2} - 191.750T^{-1}$
$\Delta Gf° = -122.361 - 15.617\times10^{-3}T\ln T + 0.591\times10^{-6}T^{2} - 95.875T^{-1} + 184.801\times10^{-3}T$

561.4-2000 K: $\Delta Hf° = -99.847 + 3.590\times10^{-3}T - 0.450\times10^{-6}T^{2} + 66.250T^{-1}$
$\Delta Gf° = -99.847 - 3.590\times10^{-3}T\ln T + 0.450\times10^{-6}T^{2} + 33.125T^{-1} + 68.232\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K and temperature and enthalpy of fusion.

$WCl_5(g)$

Tungsten Pentachloride (ideal gas)

[Formation: $W(c) + 2.5Cl_2(g) = WCl_5(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	28.736	96.935	96.935	0	-98.600	-85.455	62.639
300	28.769	97.113	96.936	.053	-98.595	-85.372	62.193
400	29.979	105.576	98.081	2.998	-98.316	-81.006	44.259
500	30.596	112.339	100.279	6.030	-98.023	-76.711	33.530
600	30.947	117.951	102.771	9.108	-97.735	-72.481	26.401
700	31.166	122.740	105.290	12.215	-97.450	-68.291	21.321
800	31.311	126.911	107.737	15.339	-97.173	-64.149	17.525
900	31.413	130.605	110.076	18.476	-96.902	-60.031	14.577
1000	31.490	133.919	112.298	21.621	-96.636	-55.951	12.228
1100	31.553	136.924	114.403	24.773	-96.380	-51.887	10.309
1200	31.608	139.671	116.395	27.931	-96.134	-47.859	8.716
1300	31.660	142.204	118.285	31.095	-95.894	-43.841	7.370
1400	31.711	144.552	120.078	34.263	-95.665	-39.836	6.219
1500	31.763	146.741	121.783	37.437	-95.442	-35.860	5.225
1600	31.817	148.793	123.408	40.616	-95.228	-31.893	4.356
1700	31.873	150.723	124.958	43.800	-95.019	-27.929	3.590
1800	31.930	152.547	126.441	46.991	-94.816	-24.003	2.914
1900	31.988	154.275	127.861	50.186	-94.619	-20.068	2.308
2000	32.047	155.917	129.223	53.388	-94.431	-16.155	1.765

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 31.464 + 0.276\times10^{-3}T - 2.498\times10^{5}T^{-2}$

$H°- H°_{298} = 31.464\times10^{-3}T + 0.138\times10^{-6}T^{2} + 2.498\times10^{2}T^{-1} - 10.231$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -99.822 + 3.581\times10^{-3}T - 0.453\times10^{-6}T^{2} + 58.050T^{-1}$

$\Delta Gf° = -99.822 - 3.581\times10^{-3}T\ln T + 0.453\times10^{-6}T^{2} + 29.025T^{-1} + 68.134\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$(WCl_5)_2(g)$

Dimeric Tungsten Pentachloride (ideal gas)

[Formation: $2W(c) + 5Cl_2(g) = (WCl_5)_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	62.969	170.521	170.521	0	-207.600	-174.348	127.799
300	63.017	170.911	170.521	.117	-207.580	-174.139	126.859
400	64.828	189.319	173.019	6.520	-206.509	-163.155	89.142
500	65.754	203.895	177.789	13.053	-205.453	-152.438	66.630
600	66.283	215.934	183.171	19.658	-204.429	-141.938	51.700
700	66.612	226.178	188.601	26.304	-203.425	-131.597	41.086
800	66.830	235.088	193.868	32.976	-202.447	-121.413	33.168
900	66.981	242.969	198.895	39.667	-201.488	-111.330	27.034
1000	67.090	250.032	203.661	46.371	-200.544	-101.366	22.153
1100	67.171	256.430	208.172	53.084	-199.622	-91.475	18.174
1200	67.233	262.278	212.441	59.805	-198.725	-81.699	14.879
1300	67.281	267.661	216.483	66.531	-197.847	-71.969	12.099
1400	67.320	272.649	220.320	73.261	-196.995	-62.300	9.725
1500	67.351	277.295	223.966	79.994	-196.164	-52.719	7.681
1600	67.377	281.642	227.435	86.731	-195.357	-43.176	5.898
1700	67.398	285.728	230.746	93.469	-194.568	-33.668	4.328
1800	67.416	289.580	233.908	100.210	-193.804	-24.253	2.945
1900	67.431	293.226	236.935	106.953	-193.057	-14.839	1.707
2000	67.444	296.685	239.837	113.696	-192.343	-5.493	.600

*Data except enthalpy of formation at 298 K estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 67.190 + 0.234\times10^{-3}T - 3.814\times10^{5}T^{-2}$

$H°- H°_{298} = 67.190\times10^{-3}T + 0.117\times10^{-6}T^{2} + 3.814\times10^{2}T^{-1} - 21.322$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -210.905 + 11.425\times10^{-3}T - 1.065\times10^{-6}T^{2} - 2.100T^{-1}$

$\Delta Gf° = -210.905 - 11.425\times10^{-3}T\ln T + 1.065\times10^{-6}T^{2} - 1.050T^{-1} + 187.402\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

WCl_6(c,l,g)
Tungsten Hexachloride
[Formation: $W(c) + 3Cl_2(g) = WCl_6(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	41.926	57.000	57.000	0	-141.900	-108.904	79.828
300	42.000	57.260	57.000	.078	-141.878	-108.698	79.185
400	46.000	69.890	58.695	4.478	-140.559	-97.829	53.451
450	48.000	75.317	60.255	6.778	-139.833	-92.535	44.940
450	50.000	77.539	60.255	7.778	-138.833	-92.535	44.940
500	50.000	82.807	62.251	10.278	-137.924	-87.439	38.219
503	50.000	83.106	62.374	10.428	-137.870	-87.136	37.860
503	45.000	90.601	62.374	14.198	-134.100	-87.136	37.860
555	45.000	95.028	65.230	16.538	-133.434	-82.318	32.415
555	48.000	97.911	65.230	18.138	-131.834	-82.318	32.415
600	48.000	101.653	67.823	20.298	-131.129	-78.331	28.532
613.6	48.000	102.729	68.585	20.951	-130.918	-77.137	27.474
613.6	36.882	126.065	68.585	35.270	-116.599	-77.137	27.474
700	37.085	130.938	75.988	38.465	-116.222	-71.604	22.355
800	37.239	135.901	83.174	42.182	-115.795	-65.265	17.829
900	37.346	140.294	89.281	45.912	-115.376	-58.967	14.319
1000	37.423	144.233	94.583	49.650	-114.965	-52.724	11.523
1100	37.481	147.802	99.260	53.396	-114.563	-46.509	9.240
1200	37.524	151.065	103.443	57.146	-114.175	-40.347	7.348
1300	37.558	154.070	107.224	60.900	-113.796	-34.205	5.750
1400	37.585	156.855	110.671	64.658	-113.429	-28.086	4.384
1500	37.607	159.449	113.838	68.417	-113.074	-22.009	3.207
1600	37.625	161.876	116.764	72.179	-112.731	-15.945	2.178
1700	37.640	164.158	119.486	75.942	-112.397	-9.895	1.272
1800	37.653	166.310	122.028	79.707	-112.076	-3.891	.472
1900	37.663	168.346	124.413	83.473	-111.764	2.120	-.244
2000	37.672	170.278	126.659	87.239	-111.470	8.098	-.885

Phase changes: 450 K, α_1 - α_2 transition point of WCl_6; ΔH° = 1.000 kcal/mol.
503 K, α_2 - β transition point of WCl_6; ΔH° = 3.770 kcal/mol.
555 K, melting point of WCl_6; ΔH° = 1.600 kcal/mol.
613.6 K, boiling point of WCl_6; ΔH° = 14.319 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-450 K: $Cp^\circ = 49.598 + 0.688\times10^{-3}T - 7.002\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 49.598\times10^{-3}T + 0.344\times10^{-6}T^2 + 7.002\times10^{2}T^{-1} - 17.167$

450-503 K: $Cp^\circ = 50.000$

$H^\circ - H^\circ_{298} = 50.000\times10^{-3}T - 14.722$

503-555 K: $Cp^\circ = 45.000$

$H^\circ - H^\circ_{298} = 45.000\times10^{-3}T - 8.437$

555-613.6 K: $Cp^\circ = 48.000$

$H^\circ - H^\circ_{298} = 48.000\times10^{-3}T - 8.502$

613.6-2000 K: $Cp^\circ = 37.750 - 3.253\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 37.750\times10^{-3}T + 3.253\times10^{2}T^{-1} + 11.576$

WCl_6(c,l,g) - Continued

Formation equations (kcal/mol):

298.15-450 K: $\Delta Hf^\circ = -148.624 + 17.302\times10^{-3}T - 0.291\times10^{-6}T^2 + 474.300T^{-1}$

$\Delta Gf^\circ = -148.624 - 17.302\times10^{-3}T\ln T + 0.291\times10^{-6}T^2 + 237.150T^{-1} + 229.046\times10^{-3}T$

450-503 K: $\Delta Hf^\circ = -146.179 + 17.704\times10^{-3}T - 0.635\times10^{-6}T^2 - 225.900T^{-1}$

$\Delta Gf^\circ = -146.179 - 17.704\times10^{-3}T\ln T + 0.635\times10^{-6}T^2 - 112.950T^{-1} + 227.643\times10^{-3}T$

503-555 K: $\Delta Hf^\circ = -139.894 + 12.704\times10^{-3}T - 0.635\times10^{-6}T^2 - 225.900T^{-1}$

$\Delta Gf^\circ = -139.894 - 12.704\times10^{-3}T\ln T + 0.635\times10^{-6}T^2 - 112.950T^{-1} + 184.045\times10^{-3}T$

555-613.6 K: $\Delta Hf^\circ = -139.959 + 15.704\times10^{-3}T - 0.635\times10^{-6}T^2 - 225.900T^{-1}$

$\Delta Gf^\circ = -139.959 - 15.704\times10^{-3}T\ln T + 0.635\times10^{-6}T^2 - 112.950T^{-1} + 203.119\times10^{-3}T$

613.6-2000 K: $\Delta Hf^\circ = -119.881 + 5.454\times10^{-3}T - 0.635\times10^{-6}T^2 + 99.400T^{-1}$

$\Delta Gf^\circ = -119.881 - 5.454\times10^{-3}T\ln T + 0.635\times10^{-6}T^2 + 49.700T^{-1} + 104.167\times10^{-3}T$

Source: Data from JANAF (60).

$WCl_6(g)$

Tungsten Hexachloride (ideal gas)

[Formation: $W(c) + 3Cl_2(g) = WCl_6(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	34.402	100.155	100.155	0	-118.000	-97.870	71.740
300	34.439	100.368	100.155	.064	-117.992	-97.744	71.206
400	35.793	110.486	101.526	3.584	-117.553	-91.061	49.753
500	36.468	118.553	104.153	7.200	-117.102	-84.490	36.930
600	36.850	125.239	107.126	10.868	-116.659	-78.013	28.416
700	37.085	130.938	110.131	14.565	-116.222	-71.604	22.355
800	37.239	135.901	113.049	18.282	-115.795	-65.265	17.829
900	37.346	140.294	115.836	22.012	-115.376	-58.967	14.319
1000	37.423	144.233	118.483	25.750	-114.965	-52.724	11.523
1100	37.481	147.802	120.987	29.496	-114.563	-46.509	9.240
1200	37.524	151.065	123.360	33.246	-114.175	-40.347	7.348
1300	37.558	154.070	125.608	37.000	-113.796	-34.205	5.750
1400	37.585	156.855	127.742	40.758	-113.429	-28.086	4.384
1500	37.607	159.449	129.771	44.517	-113.074	-22.009	3.207
1600	37.625	161.876	131.702	48.279	-112.731	-15.945	2.178
1700	37.640	164.158	133.545	52.042	-112.397	-9.896	1.272
1800	37.653	166.310	135.306	55.807	-112.076	-3.891	.472
1900	37.663	168.346	136.992	59.573	-111.764	2.120	-.244
2000	37.672	170.278	138.609	63.339	-111.470	8.098	-.885

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 37.561 + 0.118\times10^{-3}T - 2.840\times10^{5}T^{-2}$

$H°- H°_{298} = 37.561\times10^{-3}T + 0.059\times10^{-6}T^{2} + 2.840\times10^{2}T^{-1} - 12.157$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -119.713 + 5.265\times10^{-3}T - 0.576\times10^{-6}T^{2} + 58.100T^{-1}$

$\Delta Gf° = -119.713 - 5.265\times10^{-3}T\ln T + 0.576\times10^{-6}T^{2} + 29.050T^{-1} + 102.761\times10^{-3}T$

Source: Data from JANAF (60) who estimated some molecular constants.

WF(g)
Tungsten Monofluoride (ideal gas)
[Formation: $W(c) + 0.5F_2(g) = WF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	7.755	59.903	59.903	0	92.300	83.987	-61.563
300	7.764	59.951	59.904	.014	92.296	83.936	-61.147
400	8.140	62.240	60.213	.811	92.118	81.177	-44.353
500	8.386	64.085	60.809	1.638	91.937	78.462	-34.295
600	8.547	65.629	61.487	2.485	91.751	75.781	-27.603
700	8.659	66.956	62.176	3.346	91.562	73.138	-22.834
800	8.743	68.118	62.848	4.216	91.369	70.515	-19.264
900	8.811	69.151	63.491	5.094	91.170	67.926	-16.495
1000	8.872	70.083	64.105	5.978	90.969	65.354	-14.283
1100	8.930	70.931	64.687	6.868	90.763	62.811	-12.479
1200	8.985	71.711	65.241	7.764	90.552	60.271	-10.977
1300	9.040	72.432	65.767	8.665	90.336	57.763	-9.711
1400	9.094	73.104	66.267	9.572	90.114	55.275	-8.629
1500	9.146	73.733	66.744	10.484	89.889	52.790	-7.691
1600	9.197	74.325	67.199	11.401	89.658	50.326	-6.874
1700	9.247	74.884	67.635	12.323	89.424	47.883	-6.156
1800	9.295	75.414	68.052	13.251	89.185	45.436	-5.517
1900	9.342	75.918	68.454	14.182	88.941	43.014	-4.948
2000	9.389	76.398	68.839	15.119	88.693	40.599	-4.436

*Data estimated.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.453 + 0.484\times10^{-3}T - 0.748\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.453\times10^{-3}T + 0.242\times10^{-6}T^2 + 0.748\times10^{2}T^{-1} - 2.793$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf^\circ = 92.789 - 1.616\times10^{-3}T - 0.216\times10^{-6}T^2 + 3.550T^{-1}$

$\Delta Gf^\circ = 92.789 + 1.616\times10^{-3}T\ln T + 0.216\times10^{-6}T^2 + 1.775T^{-1} - 38.814\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

$WF_6(g)$

Tungsten Hexafluoride (ideal gas)

[Formation: $W(c) + 3F_2(g) = WF_6(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	28.448	81.504	81.504	0	-411.500	-390.145	285.980
300	28.523	81.680	81.504	.053	-411.500	-390.012	284.120
400	31.652	90.354	82.666	3.075	-411.376	-382.862	209.183
500	33.508	97.634	84.952	6.341	-411.128	-375.760	164.243
600	34.660	103.853	87.596	9.754	-410.823	-368.720	134.304
700	35.412	109.256	90.313	13.260	-410.487	-361.725	112.934
800	35.925	114.020	92.985	16.828	-410.137	-354.788	96.922
900	36.289	118.274	95.563	20.440	-409.779	-347.883	84.477
1000	36.556	122.112	98.029	24.083	-409.421	-341.028	74.531
1100	36.757	125.606	100.380	27.749	-409.066	-334.196	66.398
1200	36.912	128.811	102.617	31.433	-408.717	-327.412	59.629
1300	37.033	131.771	104.748	35.130	-408.374	-320.643	53.904
1400	37.131	134.519	106.777	38.839	-408.044	-313.901	49.002
1500	37.210	137.083	108.712	42.556	-407.722	-307.192	44.757
1600	37.275	139.487	110.562	46.280	-407.411	-300.497	41.046
1700	37.329	141.748	112.330	50.010	-407.107	-293.814	37.772
1800	37.374	143.883	114.024	53.746	-406.818	-287.170	34.867
1900	37.413	145.905	115.650	57.485	-406.536	-280.526	32.267
2000	37.446	147.825	117.211	61.228	-406.271	-273.909	29.931

Phase changes: 275.2 K, melting point of WF_6; $\Delta H°$ = 0.980 kcal/mol.
290.3 K, boiling point of WF_6; $\Delta H°$ = 6.465 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 35.779 + 1.222\times10^{-3}T - 6.841\times10^{5}T^{-2}$

$H°- H°_{298} = 35.779\times10^{-3}T + 0.611\times10^{-6}T^{2} + 6.841\times10^{2}T^{-1} - 13.016$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta Hf° = -414.012 + 4.440\times10^{-3}T - 0.282\times10^{-6}T^{2} + 361.600T^{-1}$

$\Delta Gf° = -414.012 - 4.440\times10^{-3}T\ln T + 0.282\times10^{-6}T^{2} + 180.800T^{-1} + 103.228\times10^{-3}T$

Source: Data from JANAF (60).

$XeF_2(g)$

Xenon Difluoride (ideal gas)

[Formation: $Xe(g) + F_2(g) = XeF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	12.933	61.998	61.998	0	-25.580	-17.537	12.855
300	12.952	62.079	61.999	.024	-25.579	-17.488	12.740
400	13.678	65.915	62.518	1.359	-25.510	-14.800	8.086
500	14.075	69.013	63.515	2.749	-25.421	-12.132	5.303
600	14.312	71.604	64.656	4.169	-25.328	-9.485	3.455
700	14.460	73.822	65.811	5.608	-25.233	-6.851	2.139
800	14.560	75.758	66.934	7.059	-25.141	-4.231	1.156
900	14.630	77.479	68.013	8.519	-25.049	-1.624	.394
1000	14.680	79.022	69.037	9.985	-24.960	.975	-.213

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 14.389 + 0.486\times10^{-3}T - 1.423\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 14.389\times10^{-3}T + 0.243\times10^{-6}T^2 + 1.423\times10^{2}T^{-1} - 4.789$

Formation equations (kcal/mol):

298.15-1000 K: $\Delta Hf^\circ = -25.999 + 0.913\times10^{-3}T + 0.069\times10^{-6}T^2 + 41.800T^{-1}$

$\Delta Gf^\circ = -25.999 - 0.913\times10^{-3}T\ln T - 0.069\times10^{-6}T^2 + 20.900T^{-1} + 33.366\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Johnson (110). Other data from Osborne (179).

$XeF_6(c,l)$

Xenon Hexafluoride

[Formation: $Xe(g) + 3F_2(g) = XeF_6(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	40.963	50.282	50.282	0	-80.820	-40.398	29.612
300	41.166	50.535	50.282	.076	-80.795	-40.147	29.247
322.63	25.860	53.596	50.407	1.029	-80.466	-37.093	25.126
322.63	77.636	57.852	50.407	2.402	-79.093	-37.093	25.126
350	109.075	65.533	51.276	4.990	-77.269	-33.598	20.979

Phase change: 322.63 K, melting point of XeF_6; ΔH° = 1.373 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-322.63 K: $Cp^\circ = 16.547 + 82.112\times10^{-3}T$

$H^\circ - H^\circ_{298} = 16.547\times10^{-3}T + 41.056\times10^{-6}T^2 - 8.583$

322.63-350 K: $Cp^\circ = 121.533 + 346.588\times10^{-3}T - 162.086\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 121.533\times10^{-3}T + 173.294\times10^{-6}T^2 + 162.086\times10^{2}T^{-1} - 105.850$

Formation equations (kcal/mol):

298.15-322.63 K: $\Delta Hf^\circ = -79.254 - 13.945\times10^{-3}T + 40.534\times10^{-6}T^2 - 301.500T^{-1}$

$\Delta Gf^\circ = -79.254 + 13.945\times10^{-3}T\ln T - 40.534\times10^{-6}T^2 - 150.750T^{-1} + 64.654\times10^{-3}T$

322.63-350 K: $\Delta Hf^\circ = -175.757 + 91.041\times10^{-3}T + 172.772\times10^{-6}T^2 + 15907.100T^{-1}$

$\Delta Gf^\circ = -175.757 - 91.041\times10^{-3}T\ln T - 172.772\times10^{-6}T^2 + 7953.550T^{-1} + 935.023\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Johnson (110). Other data from Schreiner (206).

YCl_3(c,1)

Yttrium Trichloride

[Formation: $Y(c) + 1.5Cl_2(g) = YCl_3(c,1)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	22.000	32.700	32.700	0	-239.000	-221.751	162.545
300	22.038	32.836	32.700	.041	-238.993	-221.643	161.465
400	23.430	39.391	33.583	2.323	-238.598	-215.919	117.971
500	24.168	44.706	35.294	4.706	-238.151	-210.297	91.920
600	24.646	49.157	37.244	7.148	-237.686	-204.768	74.586
700	25.002	52.984	39.225	9.631	-237.211	-199.323	62.231
800	25.293	56.342	41.160	12.146	-236.734	-193.942	52.982
900	25.546	59.336	43.016	14.688	-236.253	-188.626	45.804
994	25.763	61.885	44.682	17.100	-235.802	-183.671	40.383
994	32.400	69.450	44.682	24.620	-228.282	-183.671	40.383
1000	32.400	69.645	44.831	24.814	-228.214	-183.401	40.082
1100	32.400	72.733	47.229	28.054	-227.081	-178.982	35.560
1200	32.400	75.552	49.474	31.294	-225.972	-174.658	31.809
1300	32.400	78.146	51.581	34.534	-224.883	-170.425	28.651

*Entropy and heat capacity at 298 K estimated.

Phase change: 994 K, melting point of YCl_3; $\Delta H° = 7.520$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-994 K: $Cp° = 24.317 + 1.710\times10^{-3}T - 2.513\times10^{5}T^{-2}$

$H°- H°_{298} = 24.317\times10^{-3}T + 0.855\times10^{-6}T^2 + 2.513\times10^{2}T^{-1} - 8.169$

994-1300 K: $Cp° = 32.400$

$H°- H°_{298} = 32.400\times10^{-3}T - 7.586$

Formation equations (kcal/mol):

298.15-994 K: $\Delta Hf° = -241.105 + 5.359\times10^{-3}T - 0.182x^{-6}T^2T2 + 156.150T^{-1}$

$\Delta Gf° = -241.105 - 5.359\times10^{-3}T\ln T + 0.182\times10^{-6}T^2 + 78.075T^{-1} + 94.514\times10^{-3}T$

994-1300 K: $\Delta Hf° = -240.522 + 13.442\times10^{-3}T - 1.037\times10^{-6}T^2 - 95.150T^{-1}$

$\Delta Gf° = -240.522 - 13.442\times10^{-3}T\ln T + 1.037\times10^{-6}T^2 - 47.575T^{-1} + 148.991\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (254). Entropy and heat capacity at 298 K estimated. High-temperature data based on Dworkin (69).

YF_3(c,l)

Yttrium Trifluoride

[Formation: $Y(c,l) + 1.5F_2(g) = YF_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	20.774	21.200	21.200	0	-410.700	-392.190	287.479
300	20.834	21.329	21.202	.038	-410.695	-392.076	285.623
400	23.042	27.685	22.052	2.253	-410.275	-385.929	210.859
500	24.017	32.943	23.721	4.611	-409.780	-379.896	166.050
600	24.555	37.374	25.637	7.042	-409.267	-373.966	136.215
700	24.892	41.186	27.592	9.516	-408.756	-368.126	114.933
800	25.128	44.526	29.505	12.017	-408.257	-362.355	98.989
900	25.309	47.497	31.343	14.539	-407.768	-356.651	86.606
1000	25.461	50.171	33.093	17.078	-407.294	-350.993	76.708
1100	25.597	52.605	34.759	19.631	-406.832	-345.392	68.622
1200	25.725	54.837	36.340	22.197	-406.384	-339.825	61.890
1300	25.852	56.901	37.843	24.776	-405.945	-334.293	56.199
1350	25.916	57.878	38.567	26.070	-405.732	-331.536	53.671
1350	29.230	63.626	38.567	33.830	-397.972	-331.536	53.671
1400	29.230	64.689	39.480	35.292	-397.595	-329.082	51.371
1428	29.230	65.268	39.981	36.110	-397.387	-327.714	50.155
1428	31.950	69.949	39.981	42.795	-390.702	-327.714	50.155
1500	31.950	71.521	41.457	45.096	-389.980	-324.565	47.288
1600	31.950	73.583	43.401	48.291	-388.997	-320.235	43.741
1700	31.950	75.520	45.234	51.486	-388.033	-315.960	40.619
1752	31.950	76.482	46.147	53.147	-387.545	-313.761	39.139
1752	31.950	76.482	46.147	53.147	-388.738	-313.761	39.139
1799	31.950	77.328	46.951	54.649	-388.273	-311.763	37.874
1799	31.950	77.328	46.951	54.649	-390.997	-311.763	37.874
1800	31.950	77.346	46.968	54.681	-390.989	-311.715	37.847

Phase changes: 1350 K, α - β transition point of YF_3; $\Delta H°$ = 7.760 kcal/mol.
1428 K, melting point of YF_3; $\Delta H°$ = 6.685 kcal/mol.
1752 K, α - β transition point of Y; $\Delta H°$ = 1.193 kcal/mol.
1799 K, melting point of Y; $\Delta H°$ = 2.724 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1350 K: $Cp° = 25.538 + 0.394\times10^{-3}T - 4.340\times10^{5}T^{-2}$

$H°- H°_{298} = 25.538\times10^{-3}T + 0.197\times10^{-6}T^{2} + 4.340\times10^{2}T^{-1} - 9.087$

1350-1428 K: $Cp° = 29.231$

$H°- H°_{298} = 29.231\times10^{-3}T - 5.632$

1428-1800 K: $Cp° = 31.951$

$H°- H°_{298} = 31.951\times10^{-3}T - 2.831$

YF_3(c,l) - Continued

Formation equations (kcal/mol):

298.15-1350 K: $\Delta Hf^\circ = -413.693 + 7.058\times10^{-3}T - 0.969\times10^{-6}T^2 + 290.550T^{-1}$

$\Delta Gf^\circ = -413.693 - 7.058\times10^{-3}T\ln T + 0.969\times10^{-6}T^2 + 145.275T^{-1} + 110.413\times10^{-3}T$

1350-1428 K: $\Delta Hf^\circ = -410.238 + 10.751\times10^{-3}T - 1.166\times10^{-6}T^2 - 143.450T^{-1}$

$\Delta Gf^\circ = -410.238 - 10.751\times10^{-3}T\ln T + 1.166\times10^{-6}T^2 - 71.725T^{-1} + 134.325\times10^{-3}T$

1428-1752 K: $\Delta Hf^\circ = -407.437 + 13.471\times10^{-3}T - 1.166\times10^{-6}T^2 - 143.450T^{-1}$

$\Delta Gf^\circ = -407.437 - 13.471\times10^{-3}T\ln T + 1.166\times10^{-6}T^2 - 71.725T^{-1} + 152.122\times10^{-3}T$

1752-1799 K: $\Delta Hf^\circ = -406.775 + 10.829\times10^{-3}T - 0.261\times10^{-6}T^2 - 150.750T^{-1}$

$\Delta Gf^\circ = -406.775 - 10.829\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 - 75.375T^{-1} + 133.599\times10^{-3}T$

1799-1800 K: $\Delta Hf^\circ = -406.009 + 8.889\times10^{-3}T - 0.261\times10^{-6}T^2 - 150.750T^{-1}$

$\Delta Gf^\circ = -406.009 - 8.889\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 - 75.375T^{-1} + 118.633\times10^{-3}T$

Sources: Enthalpy of formation at 298 K, low-temperature heat capacities, and entropy at 298 K from Flotow (81). High-temperature data based on Spedding (223).

$YbCl_3(g)$

Ytterbium Trichloride (ideal gas)

[Formation: $Yb(c,l,g) + 1.5Cl_2(g) = YbCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	18.659	88.403	88.403	0	-152.700	-150.961	110.656
300	18.673	88.519	88.403	.035	-152.699	-150.950	109.966
400	19.163	93.967	89.145	1.929	-152.697	-150.369	82.157
500	19.407	98.272	90.554	3.859	-152.740	-149.779	65.468
553	19.480	100.231	91.389	4.890	-152.814	-149.462	59.068
600	19.545	101.823	92.145	5.807	-152.845	-149.176	54.336
700	19.630	104.843	93.749	7.766	-152.921	-148.556	46.381
800	19.685	107.468	95.303	9.732	-153.016	-147.932	40.413
900	19.724	109.789	96.786	11.703	-153.123	-147.286	35.765
1000	19.752	111.869	98.192	13.677	-153.246	-146.638	32.047
1033	19.759	112.510	98.639	14.329	-153.292	-146.417	30.977
1033	19.759	112.510	98.639	14.329	-153.710	-146.417	30.977
1097	19.772	113.698	99.483	15.594	-153.860	-145.955	29.078
1097	19.772	113.698	99.483	15.594	-155.690	-145.955	29.078
1100	19.773	113.752	99.522	15.653	-155.696	-145.931	28.993
1200	19.788	115.473	100.781	17.631	-155.947	-145.038	26.415
1300	19.801	117.058	101.973	19.611	-156.199	-144.110	24.227
1400	19.810	118.526	103.104	21.591	-156.454	-143.174	22.350
1467	19.815	119.452	103.829	22.919	-156.625	-142.534	21.234
1467	19.815	119.452	103.829	22.919	-187.425	-142.534	21.234
1500	19.818	119.893	104.178	23.573	-187.384	-141.522	20.620
1600	19.825	121.172	105.200	25.555	-187.261	-138.470	18.914
1700	19.830	122.374	106.176	27.537	-187.139	-135.420	17.409
1800	19.835	123.507	107.106	29.521	-187.018	-132.382	16.073
1900	19.838	124.580	107.999	31.504	-186.900	-129.350	14.878
2000	19.842	125.598	108.854	33.488	-186.786	-126.326	13.804

Phase changes: 553 K, second order transition point of Yb; $\Delta H° = 0$ kcal/mol.
1033 K, α - β transition point of Yb; $\Delta H° = 0.418$ kcal/mol.
1097 K, melting point of Yb; $\Delta H° = 1.830$ kcal/mol.
1467 K, boiling point of Yb; $\Delta H° = 30.800$ Kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.810 + 0.036\times10^{-3}T - 1.033\times10^{5}T^{-2}$

$H°- H°_{298} = 19.810\times10^{-3}T + 0.018\times10^{-6}T^{2} + 1.033\times10^{2}T^{-1} - 6.254$

$YbCl_3(g)$ - Continued

Formation equations (kcal/mol):

298.15-553 K: $\Delta Hf^\circ = -154.425 + 5.545\times10^{-3}T - 5.816\times10^{-6}T^2 + 175.550T^{-1}$

$\Delta Gf^\circ = -154.425 - 5.545\times10^{-3}T\ln T + 5.816\times10^{-6}T^2 + 87.775T^{-1} + 40.493\times10^{-3}T$

553-1033 K: $\Delta Hf^\circ = -152.804 + 0.341\times10^{-3}T - 0.808\times10^{-6}T^2 + 23.550T^{-1}$

$\Delta Gf^\circ = -152.804 - 0.341\times10^{-3}T\ln T + 0.808\times10^{-6}T^2 + 11.775T^{-1} + 7.714\times10^{-3}T$

1033-1097 K: $\Delta Hf^\circ = -151.449 - 2.071\times10^{-3}T - 0.114\times10^{-6}T^2 + 0.850T^{-1}$

$\Delta Gf^\circ = -151.449 + 2.071\times10^{-3}T\ln T + 0.114\times10^{-6}T^2 + 0.425T^{-1} - 9.610\times10^{-3}T$

1097-1467 K: $\Delta Hf^\circ = -153.119 - 2.217\times10^{-3}T - 0.114\times10^{-6}T^2 + 0.850T^{-1}$

$\Delta Gf^\circ = -153.119 + 2.217\times10^{-3}T\ln T + 0.114\times10^{-6}T^2 + 0.425T^{-1} - 9.110\times10^{-3}T$

1467-2000 K: $\Delta Hf^\circ = -189.520 + 1.601\times10^{-3}T - 0.114\times10^{-6}T^2 + 0.850T^{-1}$

$\Delta Gf^\circ = -189.520 - 1.601\times10^{-3}T\ln T + 0.114\times10^{-6}T^2 + 0.425T^{-1} + 43.540\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166) and Schumm (207). Other data based on Myers (165) and Dieke (56).

YbF_3(c,l)

Ytterbium Trifluoride

[Formation: $Yb(c,l,g) + 1.5F_2(g) = YbF_3(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	22.600	26.500	26.500	0	-375.200	-357.173	261.811
300	22.623	26.640	26.500	.042	-375.191	-357.061	260.115
400	23.604	33.292	27.402	2.356	-374.678	-351.094	191.827
500	24.294	38.637	29.131	4.753	-374.180	-345.253	150.908
553	24.574	41.100	30.161	6.049	-373.956	-342.199	135.238
600	24.822	43.115	31.098	7.210	-373.718	-339.510	123.665
700	25.255	46.974	33.097	9.714	-373.204	-333.847	104.230
800	25.641	50.372	35.048	12.259	-372.682	-328.266	89.677
900	26.023	53.414	36.923	14.842	-372.150	-322.740	78.371
1000	26.440	56.177	38.712	17.465	-371.603	-317.288	69.342
1033	26.601	57.038	39.284	18.340	-371.419	-315.495	66.748
1033	26.601	57.038	39.284	18.340	-371.837	-315.495	66.748
1097	26.912	58.645	40.366	20.052	-371.530	-312.008	62.159
1097	26.912	58.645	40.366	20.052	-373.360	-312.008	62.159
1100	26.927	58.719	40.416	20.133	-373.344	-311.842	61.956
1200	27.523	61.087	42.042	22.854	-372.839	-306.280	55.780
1259	27.939	62.418	42.966	24.490	-372.512	-303.006	52.598
1259	28.580	67.096	42.966	30.380	-366.622	-303.006	52.598
1300	28.580	68.012	43.741	31.552	-366.362	-300.938	50.592
1400	28.580	70.130	45.551	34.410	-365.733	-295.933	46.197
1435	28.580	70.836	46.160	35.410	-365.514	-294.193	44.805
1435	29.080	75.787	46.160	42.515	-358.409	-294.193	44.805
1467	29.080	76.428	46.813	43.446	-358.194	-292.762	43.614
1467	29.080	76.428	46.813	43.446	-388.994	-292.762	43.614
1500	29.080	77.075	47.472	44.405	-388.646	-290.599	42.340
1600	29.080	78.952	49.381	47.313	-387.594	-284.098	38.805
1700	29.080	80.715	51.173	50.221	-386.544	-277.658	35.695
1800	29.080	82.377	52.861	53.129	-385.501	-271.283	32.938

*Entropy and heat capacity at 298 K estimated.

Phase changes: 553 K, second order transition point of Yb; $\Delta H°$ = 0 kcal/mol.
1033 K, α - β transition point of Yb; $\Delta H°$ = 0.418 kcal/mol.
1097 K, melting point of Yb; $\Delta H°$ = 1.830 kcal/mol.
1259 K, α - β transition point of YbF_3; $\Delta H°$ = 5.890 kcal/mol.
1435 K, melting point of YbF_3; $\Delta H°$ = 7.105 kcal/mol.
1467 K, boiling point of Yb; $\Delta H°$ = 30.800 Kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1259 K: $Cp° = 22.753 + 3.914\times10^{-3}T - 1.173\times10^{5}T^{-2}$

$H°- H°_{298} = 22.753\times10^{-3}T + 1.957\times10^{-6}T^{2} + 1.173\times10^{2}T^{-1} - 7.351$

1259-1435 K: $Cp° = 28.580$

$H°- H°_{298} = 28.580\times10^{-3}T - 5.602$

1435-1800 K: $Cp° = 29.080$

$H°- H°_{298} = 29.080\times10^{-3}T + 0.785$

YbF_3(c,1) - Continued

Formation equations (kcal/mol):

298.15-553 K: $\Delta Hf^\circ = -377.991 + 8.967\times10^{-3}T - 4.006\times10^{-6}T^2 + 141.250T^{-1}$

$\Delta Gf^\circ = -377.991 - 8.967\times10^{-3}T\ln T + 4.006\times10^{-6}T^2 + 70.625T^{-1} + 118.928\times10^{-3}T$

553-1033 K: $\Delta Hf^\circ = -376.370 + 3.763\times10^{-3}T + 1.002\times10^{-6}T^2 - 10.750T^{-1}$

$\Delta Gf^\circ = -376.370 - 3.763\times10^{-3}T\ln T - 1.002\times10^{-6}T^2 - 5.375T^{-1} + 86.149\times10^{-3}T$

1033-1097 K: $\Delta Hf^\circ = -375.015 + 1.351\times10^{-3}T + 1.696\times10^{-6}T^2 - 33.450T^{-1}$

$\Delta Gf^\circ = -375.015 - 1.351\times10^{-3}T\ln T - 1.696\times10^{-6}T^2 - 16.725T^{-1} + 68.825\times10^{-3}T$

1097-1259 K: $\Delta Hf^\circ = -376.685 + 1.205\times10^{-3}T + 1.696\times10^{-6}T^2 - 33.450T^{-1}$

$\Delta Gf^\circ = -376.685 - 1.205\times10^{-3}T\ln T - 1.696\times10^{-6}T^2 - 16.725T^{-1} + 69.325\times10^{-3}T$

1259-1435 K: $\Delta Hf^\circ = -374.936 + 7.032\times10^{-3}T - 0.261\times10^{-6}T^2 - 150.750T^{-1}$

$\Delta Gf^\circ = -374.936 - 7.032\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 - 75.375T^{-1} + 107.102\times10^{-3}T$

1435-1467 K: $\Delta Hf^\circ = -368.548 + 7.532\times10^{-3}T - 0.261\times10^{-6}T^2 - 150.750T^{-1}$

$\Delta Gf^\circ = -368.548 - 7.532\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 - 75.375T^{-1} + 106.286\times10^{-3}T$

1467-1800 K: $\Delta Hf^\circ = -404.949 + 11.350\times10^{-3}T - 0.261\times10^{-6}T^2 - 150.750T^{-1}$

$\Delta Gf^\circ = -404.949 - 11.350\times10^{-3}T\ln T + 0.261\times10^{-6}T^2 - 75.375T^{-1} + 158.936\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Kim (124). Entropy and heat capacity at 298 K estimated. High-temperature data based on Spedding (222).

$YbF_3(g)$

Ytterbium Trifluoride (ideal gas)

[Formation: $Yb(c,l,g) + 1.5F_2(g) = YbF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	16.908	79.677	79.677	0	-269.100	-266.927	195.660
300	16.933	79.782	79.679	.031	-269.102	-266.915	194.445
400	17.976	84.811	80.356	1.782	-269.151	-266.176	145.430
500	18.573	88.892	81.668	3.612	-269.221	-265.422	116.014
553	18.765	90.775	82.452	4.603	-269.302	-265.016	104.735
600	18.935	92.313	83.165	5.489	-269.339	-264.650	96.397
700	19.167	95.250	84.686	7.395	-269.423	-263.859	82.379
800	19.324	97.820	86.170	9.320	-269.521	-263.063	71.865
900	19.434	100.103	87.594	11.258	-269.634	-262.245	63.681
1000	19.514	102.155	88.950	13.205	-269.763	-261.425	57.134
1033	19.534	102.789	89.382	13.849	-269.810	-261.147	55.250
1033	19.534	102.789	89.382	13.849	-270.228	-261.147	55.250
1097	19.573	103.965	90.199	15.101	-270.381	-260.574	51.912
1097	19.573	103.965	90.199	15.101	-272.211	-260.574	51.912
1100	19.575	104.018	90.236	15.160	-272.217	-260.544	51.765
1200	19.621	105.723	91.456	17.120	-272.473	-259.477	47.257
1300	19.658	107.295	92.615	19.084	-272.730	-258.374	43.436
1400	19.687	108.753	93.717	21.051	-272.992	-257.264	40.160
1467	19.702	109.674	94.424	22.371	-273.168	-256.508	38.213
1467	19.702	109.674	94.424	22.371	-303.968	-256.508	38.213
1500	19.710	110.112	94.765	23.021	-303.930	-255.438	37.217
1600	19.729	111.385	95.764	24.993	-303.814	-252.210	34.450
1700	19.746	112.581	96.718	26.967	-303.698	-248.984	32.009
1800	19.759	113.710	97.631	28.942	-303.588	-245.770	29.840
1900	19.771	114.779	98.506	30.918	-303.478	-242.562	27.901
2000	19.780	115.793	99.345	32.896	-303.373	-239.359	26.156

Phase changes: 553 K, second order transition point of Yb; ΔH° = 0 kcal/mol.
1033 K, α - β transition point of Yb; ΔH° = 0.418 kcal/mol.
1097 K, melting point of Yb; ΔH° = 1.830 kcal/mol.
1467 K, boiling point of Yb; ΔH° = 30.800 Kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.407 + 0.272\times10^{-3}T - 2.294\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.407\times10^{-3}T + 0.136\times10^{-6}T^2 + 2.294\times10^{2}T^{-1} - 6.568$

$YbF_3(g)$ - Continued

Formation equations (kcal/mol):

298.15-553 K: $\Delta Hf^\circ = -271.108 + 5.621\times10^{-3}T - 5.827\times10^{-6}T^2 + 253.350T^{-1}$

$\Delta Gf^\circ = -271.108 - 5.621\times10^{-3}T\ln T + 5.827\times10^{-6}T^2 + 126.675T^{-1} + 42.885\times10^{-3}T$

553-1033 K: $\Delta Hf^\circ = -269.486 + 0.417\times10^{-3}T - 0.819\times10^{-6}T^2 + 101.350T^{-1}$

$\Delta Gf^\circ = -269.486 - 0.417\times10^{-3}T\ln T + 0.819\times10^{-6}T^2 + 50.675T^{-1} + 10.106\times10^{-3}T$

1033-1097 K: $\Delta Hf^\circ = -268.131 - 1.995\times10^{-3}T - 0.125\times10^{-6}T^2 + 78.650T^{-1}$

$\Delta Gf^\circ = -268.131 + 1.995\times10^{-3}T\ln T + 0.125\times10^{-6}T^2 + 39.325T^{-1} - 7.218\times10^{-3}T$

1097-1467 K: $\Delta Hf^\circ = -269.801 - 2.141\times10^{-3}T - 0.125\times10^{-6}T^2 + 78.650T^{-1}$

$\Delta Gf^\circ = -269.801 + 2.141\times10^{-3}T\ln T + 0.125\times10^{-6}T^2 + 39.325T^{-1} - 6.718\times10^{-3}T$

1467-2000 K: $\Delta Hf^\circ = -306.202 + 1.677\times10^{-3}T - 0.125\times10^{-6}T^2 + 78.650T^{-1}$

$\Delta Gf^\circ = -306.202 - 1.677\times10^{-3}T\ln T + 0.125\times10^{-6}T^2 + 39.325T^{-1} + 45.933\times10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Myers (166). Other data based on Myers (165) and Dieke (56).

$ZnBr_2$(c,1)
Zinc Dibromide
[Formation: $Zn(c,1) + Br_2(l,g) = ZnBr_2(c,1)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	15.700	33.100	33.100	0	-78.550	-74.606	54.687
300	15.710	33.200	33.100	.030	-78.564	-74.580	54.331
332.6	16.052	34.838	33.191	.548	-78.833	-74.134	48.712
332.6	16.052	34.838	33.191	.548	-85.898	-74.134	48.712
400	16.760	37.860	33.735	1.650	-85.804	-71.763	39.209
500	17.800	41.710	34.950	3.380	-85.596	-68.274	29.842
600	18.840	45.050	36.367	5.210	-85.320	-64.837	23.616
675	19.610	47.320	37.460	6.655	-85.065	-62.295	20.169
675	27.200	52.860	37.460	10.395	-81.325	-62.295	20.169
692.73	27.200	53.556	37.854	10.877	-81.126	-61.791	19.494
692.73	27.200	53.556	37.854	10.877	-82.876	-61.791	19.494
700	27.200	53.840	38.019	11.075	-82.798	-61.570	19.223
800	27.200	57.480	40.236	13.795	-81.723	-58.616	16.013
900	27.200	60.680	42.330	16.515	-80.652	-55.790	13.547
1000	27.200	63.550	44.315	19.235	-79.582	-53.089	11.602

*Heat capacity at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
675 K, melting point of $ZnBr_2$; $\Delta H°$ = 3.740 kcal/mol.
692.73 K, melting point of Zn; $\Delta H°$ = 1.750 kcal/mol.

Heat capacity (cal/mol ·K) and enthalpy (kcal/mol) equations:

298.15-675 K: $Cp° = 12.600 + 10.400\times10^{-3}T$
$H°- H°_{298} = 12.600\times10^{-3}T + 5.200\times10^{-6}T^2 - 4.219$
675-1000 K: $Cp° = 27.200$
$H°- H°_{298} = 27.200\times10^{-3}T - 7.965$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -75.782 - 10.590\times10^{-3}T + 3.908\times10^{-6}T^2 + 12.600T^{-1}$
$\Delta Gf° = -75.782 + 10.590\times10^{-3}T\ln T - 3.908\times10^{-6}T^2 + 6.300T^{-1} - 55.297\times10^{-3}T$
332.6-675 K: $\Delta Hf° = -85.783 - 1.429\times10^{-3}T + 3.753\times10^{-6}T^2 - 18.800T^{-1}$
$\Delta Gf° = -85.783 + 1.429\times10^{-3}T\ln T - 3.753\times10^{-6}T^2 - 9.400T^{-1} + 28.058\times10^{-3}T$
675-692.73 K: $\Delta Hf° = -89.528 + 13.171\times10^{-3}T - 1.447\times10^{-6}T^2 - 18.800T^{-1}$
$\Delta Gf° = -89.528 - 13.171\times10^{-3}T\ln T + 1.447\times10^{-6}T^2 - 9.400T^{-1} + 125.212\times10^{-3}T$
692.73-1000 K: $\Delta Hf° = -90.265 + 10.770\times10^{-3}T - 0.055\times10^{-6}T^2 - 31.400T^{-1}$
$\Delta Gf° = -90.265 - 10.770\times10^{-3}T\ln T + 0.055\times10^{-6}T^2 - 15.700T^{-1} + 111.548\times10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from Wagman (252). High-temperature data based on Cubicciotti (46).

$ZnCl_2(c,l)$
Zinc Dichloride
[Formation: $Zn(c,l) + Cl_2(g) = ZnCl_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	17.050	26.645	26.645	0	-99.200	-88.289	64.717
300	17.070	26.751	26.651	.030	-99.196	-88.223	64.270
400	17.880	31.781	27.331	1.780	-98.894	-84.610	46.228
500	18.490	35.839	28.639	3.600	-98.567	-81.077	35.438
570	18.880	38.287	29.673	4.910	-98.327	-78.642	30.152
570	18.890	42.375	29.673	7.240	-95.997	-78.642	30.152
600	19.060	43.348	30.331	7.810	-95.892	-77.730	28.313
692.73	19.570	46.122	32.268	9.598	-95.563	-74.954	23.647
692.73	19.570	46.122	32.268	9.598	-97.313	-74.954	23.647
700	19.610	46.327	32.413	9.740	-97.290	-74.718	23.328

Phase changes: 570 K, melting point of $ZnCl_2$; $\Delta H° = 2.330$ kcal/mol.
629.73 K, melting point of Zn; $\Delta H° = 1.750$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-570 K: $Cp° = 16.236 + 5.032\times10^{-3}T - 0.610\times10^{5}T^{-2}$
$H°- H°_{298} = 16.236\times10^{-3}T + 2.516\times10^{-6}T^2 + 0.610\times10^{2}T^{-1} - 5.269$
570-700 K: $Cp° = 15.735 + 5.528\times10^{-3}T$
$H°- H°_{298} = 15.735\times10^{-3}T + 2.764\times10^{-6}T^2 - 2.627$

Formation equations (kcal/mol):

298.15-570 K: $\Delta Hf° = -99.999 + 2.310\times10^{-3}T + 1.036\times10^{-6}T^2 + 5.300T^{-1}$
$\Delta Gf° = -99.999 - 2.310\times10^{-3}T\ln T - 1.036\times10^{-6}T^2 + 2.650T^{-1} + 52.714\times10^{-3}T$
570-692.73 K: $\Delta Hf° = -97.357 + 1.809\times10^{-3}T + 1.284\times10^{-6}T^2 - 55.700T^{-1}$
$\Delta Gf° = -97.357 - 1.809\times10^{-3}T\ln T - 1.284\times10^{-6}T^2 - 27.850T^{-1} + 45.135\times10^{-3}T$
692.73-700 K: $\Delta Hf° = -98.093 - 0.592\times10^{-3}T + 2.676\times10^{-6}T^2 - 68.300T^{-1}$
$\Delta Gf° = -98.093 + 0.592\times10^{-3}T\ln T - 2.676\times10^{-6}T^2 - 34.150T^{-1} + 31.472\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Low-temperature heat capacities and entropy of formation at 298 K from McBride (156). High-temperature data based on Angell (5) and Cubicciotti (46).

ZnF_2(c,l)
Zinc Difluoride
[Formation: $Zn(c,l,g) + F_2(g) = ZnF_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	15.690	17.610	17.610	0	-182.700	-170.541	125.008
300*	15.720	17.707	17.610	.029	-182.696	-170.465	124.182
400	17.000	22.419	18.244	1.670	-182.442	-166.424	90.928
500	17.890	26.312	19.480	3.416	-182.140	-162.454	71.008
600	18.610	29.639	20.902	5.242	-181.810	-158.547	57.750
692.73	19.213	32.357	22.258	6.996	-181.487	-154.979	48.894
692.73	19.213	32.357	22.258	6.996	-183.237	-154.979	48.894
700	19.260	32.558	22.364	7.136	-183.214	-154.682	48.293
800	19.890	35.171	23.804	9.094	-182.868	-150.629	41.149
900	20.500	37.549	25.200	11.114	-182.469	-146.621	35.604
1000	21.120	39.741	26.546	13.195	-182.018	-142.663	31.179
1090	21.670	41.584	27.712	15.120	-181.565	-139.140	27.898
1090	21.700	42.272	27.712	15.870	-180.815	-139.140	27.898
1100	21.770	42.471	27.846	16.087	-180.762	-138.758	27.568
1180	22.282	44.016	28.890	17.849	-180.312	-135.716	25.136
1180	22.282	44.016	28.890	17.849	-207.877	-135.716	25.136
1200	22.410	44.392	29.145	18.296	-207.709	-134.496	24.495
1220	22.530	44.763	29.398	18.745	-207.538	-133.277	23.875
1220	24.000	52.583	29.398	28.285	-197.998	-133.277	23.875
1300	24.000	54.107	30.872	30.205	-197.192	-129.059	21.697
1400	24.000	55.886	32.597	32.605	-196.189	-123.857	19.335
1500	24.000	57.542	34.205	35.005	-195.189	-118.726	17.298

*Heat capacities above 298 K estimated.

Phase changes: 692.73 K, melting point of Zn; ΔH° = 1.750 kcal/mol.
1090 K, transition point of ZnF_2; ΔH° = 0.750 kcal/mol.
1180 K, boiling point of Zn; ΔH° = 27.565 kcal/mol.
1220 K, melting point of ZnF_2; ΔH° = 9.540 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1090 K: $Cp^\circ = 15.659 + 5.594\times10^{-3}T - 1.455\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 15.659\times10^{-3}T + 2.797\times10^{-6}T^2 + 1.455\times10^{2}T^{-1} - 5.405$

1090-1220 K: $Cp^\circ = 14.730 + 6.394\times10^{-3}T$

$H^\circ - H^\circ_{298} = 14.730\times10^{-3}T + 3.197\times10^{-6}T^2 - 3.984$

1220-1500 K: $Cp^\circ = 24.000$

$H^\circ - H^\circ_{298} = 24.000\times10^{-3}T - 0.995$

ZnF_2(c,l) - Continued

Formation equations (kcal/mol):

298.15-692.73 K: $\Delta Hf^\circ = -183.614 + 2.052\times10^{-3}T + 1.231\times10^{-6}T^2 + 57.600T^{-1}$

$\Delta Gf^\circ = -183.614 - 2.052\times10^{-3}T\ln T - 1.231\times10^{-6}T^2 + 28.800T^{-1} + 55.584\times10^{-3}T$

692.73-1090 K: $\Delta Hf^\circ = -184.351 - 0.349\times10^{-3}T + 2.623\times10^{-6}T^2 + 45.000T^{-1}$

$\Delta Gf^\circ = -184.351 + 0.349\times10^{-3}T\ln T - 2.623\times10^{-6}T^2 + 22.500T^{-1} + 41.921\times10^{-3}T$

1090-1180 K: $\Delta Hf^\circ = -182.930 - 1.278\times10^{-3}T + 3.023\times10^{-6}T^2 - 100.500T^{-1}$

$\Delta Gf^\circ = -182.930 + 1.278\times10^{-3}T\ln T - 3.023\times10^{-6}T^2 - 50.250T^{-1} + 34.617\times10^{-3}T$

1180-1220 K: $\Delta Hf^\circ = -213.483 + 1.254\times10^{-3}T + 3.023\times10^{-6}T^2 - 100.500T^{-1}$

$\Delta Gf^\circ = -213.483 - 1.254\times10^{-3}T\ln T - 3.023\times10^{-6}T^2 - 50.250T^{-1} + 78.419\times10^{-3}T$

1220-1500 K: $\Delta Hf^\circ = -210.494 + 10.524\times10^{-3}T - 0.174\times10^{-6}T^2 - 100.500T^{-1}$

$\Delta Gf^\circ = -210.494 - 10.524\times10^{-3}T\ln T + 0.174\times10^{-6}T^2 - 50.250T^{-1} + 137.947\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (252). Low-temperature heat capacities and entropy at 298 K from Stout (227). Temperature and enthalpy of transition from Rimai (197). Temperature and enthalpy of fusion from Kleppa (132). Other high-temperature data derived from estimated heat capacities.

ZrBr(g)

Zirconium Monobromide (ideal gas)

[Formation: $Zr(c) + 0.5Br_2(l,g) = ZrBr(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	8.620	63.443	63.443	0	72.000	61.286	-44.924
300	8.624	63.496	63.443	.016	71.989	61.221	-44.599
332.6	8.674	64.388	63.492	.298	71.773	60.062	-39.466
332.6	8.674	64.388	63.492	.298	68.240	60.062	-39.466
400	8.776	66.000	63.783	.887	68.099	58.416	-31.917
500	8.875	67.969	64.431	1.769	67.872	56.021	-24.486
600	8.973	69.596	65.159	2.662	67.630	53.674	-19.550
700	9.086	70.987	65.894	3.565	67.373	51.368	-16.038
800	9.215	72.209	66.609	4.480	67.106	49.099	-13.413
900	9.353	73.302	67.293	5.408	66.830	46.865	-11.380
1000	9.492	74.295	67.945	6.350	66.547	44.661	-9.761
1100	9.626	75.206	68.564	7.306	66.258	42.487	-8.441
1136	9.671	75.517	68.780	7.653	66.152	41.710	-8.024
1136	9.671	75.517	68.780	7.653	65.201	41.710	-8.024
1200	9.751	76.049	69.153	8.275	65.103	40.391	-7.356
1300	9.865	76.834	69.714	9.256	64.944	38.337	-6.445
1400	9.968	77.569	70.249	10.248	64.781	36.298	-5.666
1500	10.058	78.260	70.761	11.249	64.609	34.268	-4.993
1600	10.136	78.911	71.249	12.259	64.430	32.253	-4.405
1700	10.203	79.528	71.719	13.276	64.241	30.246	-3.888
1800	10.260	80.113	72.169	14.299	64.041	28.251	-3.430
1900	10.308	80.669	72.602	15.328	63.831	26.269	-3.022
2000	10.348	81.199	73.019	16.360	63.607	24.296	-2.655

*Data estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.281 + 1.184\times10^{-3}T - 0.012\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.281\times10^{-3}T + 0.592\times10^{-6}T^2 + 0.012\times10^{2}T^{-1} - 2.526$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = 74.148 - 6.757\times10^{-3}T - 0.300\times10^{-6}T^2 - 31.700T^{-1}$

$\Delta Gf^\circ = 74.148 + 6.757\times10^{-3}T\ln T + 0.300\times10^{-6}T^2 - 15.850T^{-1} - 81.550\times10^{-3}T$

332.6-1136 K: $\Delta Hf^\circ = 69.148 - 2.177\times10^{-3}T - 0.377\times10^{-6}T^2 - 47.400T^{-1}$

$\Delta Gf^\circ = 69.148 + 2.177\times10^{-3}T\ln T + 0.377\times10^{-6}T^2 - 23.700T^{-1} - 39.872\times10^{-3}T$

1136-2000 K: $\Delta Hf^\circ = 66.652 - 1.008\times10^{-3}T - 0.246\times10^{-6}T^2 + 7.100T^{-1}$

$\Delta Gf^\circ = 66.652 + 1.008\times10^{-3}T\ln T + 0.246\times10^{-6}T^2 + 3.550T^{-1} - 29.323\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

$ZrBr_2(c,l,g)$
Zirconium Dibromide
[Formation: $Zr(c) + Br_2(l,g) = ZrBr_2(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	20.727	27.700	27.700	0	-96.700	-91.334	66.948
300	20.732	27.828	27.701	.038	-96.706	-91.300	66.511
332.6	20.821	29.971	27.821	.715	-96.820	-90.707	59.602
332.6	20.821	29.971	27.821	.715	-103.885	-90.707	59.602
400	21.006	33.830	28.518	2.125	-103.501	-88.076	48.122
500	21.280	38.547	30.067	4.240	-102.935	-84.284	36.840
600	21.554	42.451	31.816	6.381	-102.374	-80.608	29.361
700	21.828	45.794	33.580	8.550	-101.811	-77.025	24.048
800	22.102	48.727	35.293	10.747	-101.244	-73.522	20.085
900	22.376	51.345	36.934	12.970	-100.674	-70.091	17.020
900	21.750	68.012	36.934	27.970	-85.674	-70.091	17.020
1000	21.750	70.304	40.159	30.145	-85.174	-68.388	14.946
1100	21.750	72.377	42.995	32.320	-84.695	-66.732	13.258
1136	21.750	73.077	43.937	33.103	-84.528	-66.147	12.726
1136	21.750	73.077	43.937	33.103	-85.479	-66.147	12.726
1200	21.750	74.269	45.523	34.495	-85.096	-65.067	11.850
1300	21.750	76.010	47.802	36.670	-84.513	-63.423	10.662
1400	21.750	77.622	49.876	38.845	-83.946	-61.820	9.650
1500	21.750	79.123	51.776	41.020	-83.398	-60.261	8.780
1555.1	21.750	79.907	52.759	42.218	-83.104	-59.415	8.350
1555.1	15.144	100.148	52.759	73.695	-51.627	-59.415	8.350
1600	15.178	100.580	54.095	74.376	-51.686	-59.640	8.146
1700	15.260	101.502	56.856	75.898	-51.825	-60.133	7.731
1800	15.349	102.377	59.361	77.428	-51.973	-60.618	7.360
1900	15.441	103.210	61.648	78.967	-52.129	-61.095	7.027
2000	15.536	104.004	63.746	80.516	-52.293	-61.563	6.727

*Data estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
900 K, melting point of $ZrBr_2$; ΔH° = 15.000 kcal/mol.
1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.
1555.1 K, boiling point of $ZrBr_2$; ΔH° = 31.477 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-900 K: $Cp^\circ = 19.909 + 2.738\times10^{-3}T + 0.001\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 19.909\times10^{-3}T + 1.369\times10^{-6}T^2 - 0.001\times10^{2}T^{-1} - 6.057$

900-1555.1 K: $Cp^\circ = 21.750$
$H^\circ - H^\circ_{298} = 21.750\times10^{-3}T + 8.395$

1555.1-2000 K: $Cp^\circ = 15.701 + 0.112\times10^{-3}T - 17.683\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 15.701\times10^{-3}T + 0.056\times10^{-6}T^2 + 17.683\times10^{2}T^{-1} + 48.006$

$ZrBr_2$(c,l,g) - Continued

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -95.391 - 4.175\times10^{-3}T + 0.527\times10^{-6}T^2 - 33.000T^{-1}$

$\Delta Gf^\circ = -95.391 + 4.175\times10^{-3}T\ln T - 0.527\times10^{-6}T^2 - 16.500T^{-1} - 9.835\times10^{-3}T$

332.6-900 K: $\Delta Hf^\circ = -105.392 + 4.986\times10^{-3}T + 0.372\times10^{-6}T^2 - 64.400T^{-1}$

$\Delta Gf^\circ = -105.392 - 4.986\times10^{-3}T\ln T - 0.372\times10^{-6}T^2 - 32.200T^{-1} + 73.520\times10^{-3}T$

900-1136 K: $\Delta Hf^\circ = -90.940 + 6.827\times10^{-3}T - 0.997\times10^{-6}T^2 - 64.300T^{-1}$

$\Delta Gf^\circ = -90.940 - 6.827\times10^{-3}T\ln T + 0.997\times10^{-6}T^2 - 32.150T^{-1} + 68.754\times10^{-3}T$

1136-1555.1 K: $\Delta Hf^\circ = -93.436 + 7.996\times10^{-3}T - 0.866\times10^{-6}T^2 - 9.800T^{-1}$

$\Delta Gf^\circ = -93.436 - 7.996\times10^{-3}T\ln T + 0.866\times10^{-6}T^2 - 4.900T^{-1} + 79.303\times10^{-3}T$

1555.1-2000 K: $\Delta Hf^\circ = -53.825 + 1.947\times10^{-3}T - 0.810\times10^{-6}T^2 + 1758.500T^{-1}$

$\Delta Gf^\circ = -53.825 - 1.947\times10^{-3}T\ln T + 0.810\times10^{-6}T^2 + 879.250T^{-1} + 9.097\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

$ZrBr_2(g)$

Zirconium Dibromide (ideal gas)

[Formation: $Zr(c) + Br_2(l,g) = ZrBr_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	14.504	75.684	75.684	0	-41.700	-50.640	37.120
300	14.509	75.774	75.684	.027	-41.717	-50.694	36.930
332.6	14.563	77.274	75.768	.501	-42.035	-51.654	33.941
332.6	14.563	77.274	75.768	.501	-49.100	-51.654	33.941
400	14.676	79.974	76.257	1.487	-49.139	-52.172	28.505
500	14.756	83.258	77.340	2.959	-49.216	-52.921	23.131
600	14.801	85.953	78.558	4.437	-49.318	-53.653	19.543
700	14.828	88.237	79.781	5.919	-49.442	-54.366	16.974
800	14.847	90.218	80.964	7.403	-49.588	-55.059	15.041
900	14.864	91.968	82.092	8.888	-49.756	-55.734	13.534
1000	14.883	93.535	83.159	10.376	-49.943	-56.388	12.323
1100	14.908	94.955	84.169	11.865	-50.150	-57.023	11.329
1136	14.920	95.435	84.518	12.402	-50.229	-57.247	11.013
1136	14.920	95.435	84.518	12.402	-51.180	-57.247	11.013
1200	14.941	96.253	85.122	13.357	-51.234	-57.586	10.488
1300	14.984	97.451	86.025	14.854	-51.329	-58.112	9.769
1400	15.039	98.563	86.881	16.355	-51.436	-58.628	9.152
1500	15.103	99.603	87.695	17.862	-51.556	-59.139	8.616
1600	15.178	100.580	88.470	19.376	-51.686	-59.640	8.146
1700	15.260	101.502	89.209	20.898	-51.825	-60.133	7.731
1800	15.349	102.377	89.917	22.428	-51.973	-60.618	7.360
1900	15.441	103.210	90.596	23.967	-52.129	-61.095	7.027
2000	15.536	104.004	91.246	25.516	-52.293	-61.563	6.727

*Data estimated.

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H°$ = 7.065 kcal/mol.
1136 K, α - β transition point of Zr; $\Delta H°$ = 0.951 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 14.698 + 0.268\times10^{-3}T - 0.244\times10^{5}T^{-2}$

$H°- H°_{298} = 14.698\times10^{-3}T + 0.134\times10^{-6}T^2 + 0.244\times10^{2}T^{-1} - 4.476$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -38.810 - 9.386\times10^{-3}T - 0.708\times10^{-6}T^2 - 8.500T^{-1}$

$\Delta Gf° = -38.810 + 9.386\times10^{-3}T\ln T + 0.708\times10^{-6}T^2 - 4.250T^{-1} - 93.319\times10^{-3}T$

332.6-1136 K: $\Delta Hf° = -48.811 - 0.225\times10^{-3}T - 0.863\times10^{-6}T^2 - 39.900T^{-1}$

$\Delta Gf° = -48.811 + 0.225\times10^{-3}T\ln T + 0.863\times10^{-6}T^2 - 19.950T^{-1} - 9.964\times10^{-3}T$

1136-2000 K: $\Delta Hf° = -51.307 + 0.944\times10^{-3}T - 0.732\times10^{-6}T^2 + 14.600T^{-1}$

$\Delta Gf° = -51.307 - 0.944\times10^{-3}T\ln T + 0.732\times10^{-6}T^2 + 7.300T^{-1} + 0.586\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

$ZrBr_3(c)$

Zirconium Tribromide

[Formation: $Zr(c) + 1.5Br_2(l,g) = ZrBr_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	23.777	41.122	41.122	0	-152.000	-145.212	106.442
300	23.796	41.269	41.122	.044	-152.016	-145.169	105.754
332.6	24.026	43.736	41.260	.823	-152.323	-144.409	94.889
332.6	24.026	43.736	41.260	.823	-162.920	-144.409	94.889
400	24.500	48.226	42.066	2.464	-162.600	-140.694	76.870
500	24.800	53.733	43.869	4.932	-162.121	-135.273	59.127
600	25.000	58.274	45.902	7.423	-161.654	-129.947	47.333
700	25.100	62.136	47.952	9.929	-161.201	-124.698	38.932

*Data estimated.

Phase change: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp^\circ = 25.433 - 0.052\times10^{-3}T - 1.458\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.433\times10^{-3}T - 0.026\times10^{-6}T^2 + 1.458\times10^{2}T^{-1} - 8.070$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -150.011 - 7.696\times10^{-3}T - 0.818\times10^{-6}T^2 + 112.900T^{-1}$

$\Delta Gf^\circ = -150.011 + 7.696\times10^{-3}T\ln T + 0.818\times10^{-6}T^2 + 56.450T^{-1} - 28.634\times10^{-3}T$

332.6-700 K: $\Delta Hf^\circ = -165.012 + 6.045\times10^{-3}T - 1.050\times10^{-6}T^2 + 65.800T^{-1}$

$\Delta Gf^\circ = -165.012 - 6.045\times10^{-3}T\ln T + 1.050\times10^{-6}T^2 + 32.900T^{-1} + 96.398\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

$ZrBr_3(g)$

Zirconium Tribromide (ideal gas)

[Formation: $Zr(c) + 1.5Br_2(l,g) = ZrBr_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	18.988	88.787	88.787	0	-103.000	-110.423	80.942
300	18.998	88.905	88.788	.035	-103.025	-110.469	80.475
332.6	19.118	90.871	88.898	.656	-103.490	-111.254	73.103
332.6	19.118	90.871	88.898	.656	-114.088	-111.254	73.103
400	19.365	94.427	89.537	1.956	-114.107	-110.682	60.473
500	19.543	98.770	90.966	3.902	-114.151	-109.821	48.002
600	19.642	102.342	92.572	5.862	-114.215	-108.949	39.684
700	19.702	105.375	94.191	7.829	-114.301	-108.065	33.739
800	19.742	108.009	95.757	9.802	-114.406	-107.167	29.276
900	19.769	110.336	97.250	11.777	-114.533	-106.256	25.802
1000	19.789	112.420	98.665	13.755	-114.680	-105.329	23.019
1100	19.803	114.306	100.001	15.735	-114.847	-104.384	20.739
1136	19.807	114.944	100.465	16.448	-114.913	-104.041	20.016
1136	19.807	114.944	100.465	16.448	-115.864	-104.041	20.016
1200	19.814	116.030	101.267	17.716	-115.894	-103.373	18.826
1300	19.823	117.616	102.464	19.698	-115.956	-102.328	17.203
1400	19.830	119.086	103.600	21.680	-116.035	-101.276	15.810
1500	19.835	120.454	104.679	23.663	-116.133	-100.220	14.602
1600	19.840	121.734	105.705	25.647	-116.248	-99.154	13.544
1700	19.843	122.937	106.683	27.631	-116.380	-98.084	12.609
1800	19.847	124.071	107.618	29.616	-116.528	-97.003	11.778
1900	19.849	125.145	108.513	31.601	-116.694	-95.913	11.032
2000	19.852	126.163	109.370	33.586	-116.879	-94.816	10.361

*Data estimated.

Phase changes: 332.6 K, boiling point of Br_2; ΔH° = 7.065 kcal/mol.
1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.839 + 0.022\times10^{-3}T - 0.762\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.839\times10^{-3}T + 0.011\times10^{-6}T^2 + 0.762\times10^{2}T^{-1} - 6.172$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf^\circ = -99.113 - 13.290\times10^{-3}T - 0.781\times10^{-6}T^2 + 43.300T^{-1}$

$\Delta Gf^\circ = -99.113 + 13.290\times10^{-3}T\ln T + 0.781\times10^{-6}T^2 + 21.650T^{-1} - 114.135\times10^{-3}T$

332.6-1136 K: $\Delta Hf^\circ = -114.114 + 0.451\times10^{-3}T - 1.013\times10^{-6}T^2 - 3.800T^{-1}$

$\Delta Gf^\circ = -114.114 - 0.451\times10^{-3}T\ln T + 1.013\times10^{-6}T^2 - 1.900T^{-1} + 10.898\times10^{-3}T$

1136-2000 K: $\Delta Hf^\circ = -116.610 + 1.620\times10^{-3}T - 0.882\times10^{-6}T^2 + 50.700T^{-1}$

$\Delta Gf^\circ = -116.610 - 1.620\times10^{-3}T\ln T + 0.882\times10^{-6}T^2 + 25.350T^{-1} + 21.447\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

$ZrBr_4(c,g)$

Zirconium Tetrabromide

[Formation: $Zr(c) + 2Br_2(l,g) = ZrBr_4(c,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°-H°_{298})/T$	$H°-H°_{298}$	ΔHf°	ΔGf°	
298.15*	29.829	53.702	53.702	0	-181.800	-173.340	127.060
300	29.856	53.887	53.704	.055	-181.822	-173.286	126.237
332.6	30.196	56.984	53.876	1.034	-182.223	-172.338	113.241
332.6	30.196	56.984	53.876	1.034	-196.353	-172.338	113.241
400	30.900	62.630	54.888	3.097	-195.904	-167.520	91.528
500	31.460	69.588	57.156	6.216	-195.216	-160.504	70.155
600	31.870	75.362	59.724	9.383	-194.517	-153.627	55.958
628.5	31.960	76.842	60.465	10.293	-194.316	-151.688	52.746
628.5	25.515	117.781	60.465	36.023	-168.586	-151.688	52.746
700	25.579	120.534	66.464	37.849	-168.550	-149.770	46.760
800	25.638	123.954	73.442	40.410	-168.514	-147.089	40.182
900	25.678	126.976	79.225	42.976	-168.500	-144.412	35.068
1000	25.707	129.683	84.137	45.546	-168.505	-141.736	30.976
1100	25.729	132.134	88.391	48.117	-168.532	-139.057	27.628
1136	25.735	132.963	89.791	49.043	-168.547	-138.093	26.567
1136	25.735	132.963	89.791	49.043	-169.498	-138.093	26.567
1200	25.746	134.374	92.131	50.691	-169.437	-136.324	24.828
1300	25.758	136.435	95.461	53.266	-169.359	-133.570	22.455
1400	25.769	138.344	98.456	55.843	-169.296	-130.816	20.421
1500	25.777	140.122	101.175	58.420	-169.254	-128.070	18.660
1600	25.784	141.786	103.662	60.998	-169.229	-125.325	17.118
1700	25.789	143.349	105.951	63.577	-169.221	-122.583	15.759
1800	25.794	144.824	108.071	66.156	-169.231	-119.841	14.550
1900	25.798	146.218	110.041	68.736	-169.258	-117.092	13.468
2000	25.801	147.542	111.884	71.316	-169.305	-114.349	12.495

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.
628.5 K, sublimation point of $ZrBr_4$; $\Delta H° = 25.730$ kcal/mol.
1136 K, α - β transition point of Zr; $\Delta H° = 0.951$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-628.5 K:
$$Cp° = 30.983 + 2.244\times10^{-3}T - 1.621\times10^{5}T^{-2}$$
$$H°-H°_{298} = 30.983\times10^{-3}T + 1.122\times10^{-6}T^{2} + 1.621\times10^{2}T^{-1} - 9.881$$

628.5-2000 K:
$$Cp° = 25.819 + 0.010\times10^{-3}T - 1.222\times10^{5}T^{-2}$$
$$H°-H°_{298} = 25.819\times10^{-3}T + 0.005\times10^{-6}T^{2} + 1.222\times10^{2}T^{-1} + 19.599$$

Formation equations (kcal/mol):

298.15-332.6 K:
$$\Delta Hf° = -178.930 - 11.192\times10^{-3}T + 0.380\times10^{-6}T^{2} + 129.200T^{-1}$$
$$\Delta Gf° = -178.930 + 11.192\times10^{-3}T\ln T - 0.380\times10^{-6}T^{2} + 64.600T^{-1} - 45.630\times10^{-3}T$$

332.6-628.5 K:
$$\Delta Hf° = -198.931 + 7.130\times10^{-3}T + 0.070\times10^{-6}T^{2} + 66.400T^{-1}$$
$$\Delta Gf° = -198.931 - 7.130\times10^{-3}T\ln T - 0.070\times10^{-6}T^{2} + 33.200T^{-1} + 121.080\times10^{-3}T$$

628.5-1136 K:
$$\Delta Hf° = -169.451 + 1.966\times10^{-3}T - 1.047\times10^{-6}T^{2} + 26.500T^{-1}$$
$$\Delta Gf° = -169.451 - 1.966\times10^{-3}T\ln T + 1.047\times10^{-6}T^{2} + 13.250T^{-1} + 40.249\times10^{-3}T$$

1136-2000 K:
$$\Delta Hf° = -171.947 + 3.135\times10^{-3}T - 0.916\times10^{-6}T^{2} + 81.000T^{-1}$$
$$\Delta Gf° = -171.947 - 3.135\times10^{-3}T\ln T + 0.916\times10^{-6}T^{2} + 40.500T^{-1} + 50.798\times10^{-3}T$$

Source: Data from Chase (26) who estimated all except enthalpy of formation at 298 K.

$ZrBr_4(g)$

Zirconium Tetrabromide (ideal gas)

[Formation: $Zr(c) + 2Br_2(l,g) = ZrBr_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	24.538	99.037	99.037	0	-154.100	-159.156	116.663
300	24.553	99.189	99.039	.045	-154.132	-159.187	115.966
332.6	24.726	101.731	99.180	.848	-154.709	-159.707	104.941
332.6	24.726	101.731	99.180	.848	-168.839	-159.707	104.941
400	25.083	106.335	100.007	2.531	-168.770	-157.868	86.254
500	25.343	111.963	101.857	5.053	-168.679	-155.155	67.817
600	25.489	116.598	103.938	7.596	-168.604	-152.456	55.531
700	25.579	120.534	106.035	10.149	-168.550	-149.770	46.760
800	25.638	123.954	108.067	12.710	-168.514	-147.089	40.182
900	25.678	126.976	110.003	15.276	-168.500	-144.412	35.068
1000	25.707	129.683	111.837	17.846	-168.505	-141.736	30.976
1100	25.729	132.134	113.573	20.417	-168.532	-139.058	27.628
1136	25.735	132.963	114.174	21.343	-168.547	-138.093	26.567
1136	25.735	132.963	114.174	21.343	-169.498	-138.093	26.567
1200	25.746	134.374	115.215	22.991	-169.437	-136.324	24.828
1300	25.758	136.435	116.769	25.566	-169.359	-133.570	22.455
1400	25.769	138.344	118.242	28.143	-169.296	-130.816	20.421
1500	25.777	140.122	119.642	30.720	-169.254	-128.070	18.660
1600	25.784	141.786	120.975	33.298	-169.229	-125.325	17.118
1700	25.789	143.349	122.245	35.877	-169.221	-122.583	15.759
1800	25.794	144.824	123.460	38.456	-169.231	-119.841	14.550
1900	25.798	146.218	124.620	41.036	-169.258	-117.092	13.468
2000	25.801	147.542	125.734	43.616	-169.305	-114.349	12.495

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 332.6 K, boiling point of Br_2; $\Delta H° = 7.065$ kcal/mol.
1136 K, α - β transition point of Zr; $\Delta H° = 0.951$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 25.771 + 0.038\times10^{-3}T - 1.106\times10^{5}T^{-2}$

$H°- H°_{298} = 25.771\times10^{-3}T + 0.019\times10^{-6}T^2 + 1.106\times10^{2}T^{-1} - 8.056$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta Hf° = -149.405 - 16.404\times10^{-3}T - 0.723\times10^{-6}T^2 + 77.700T^{-1}$

$\Delta Gf° = -149.405 + 16.404\times10^{-3}T\ln T + 0.723\times10^{-6}T^2 + 38.850T^{-1} - 126.820\times10^{-3}T$

332.6-1136 K: $\Delta Hf° = -169.406 + 1.918\times10^{-3}T - 1.033\times10^{-6}T^2 + 14.900T^{-1}$

$\Delta Gf° = -169.406 - 1.918\times10^{-3}T\ln T + 1.033\times10^{-6}T^2 + 7.450T^{-1} + 39.890\times10^{-3}T$

1136-2000 K: $\Delta Hf° = -171.902 + 3.087\times10^{-3}T - 0.902\times10^{-6}T^2 + 69.400T^{-1}$

$\Delta Gf° = -171.902 - 3.087\times10^{-3}T\ln T + 0.902\times10^{-6}T^2 + 34.700T^{-1} + 50.439\times10^{-3}T$

Source: Data from Chase (26) who estimated all except enthalpy of formation at 298 K.

ZrCl(g)

Zirconium Monochloride (ideal gas)

[Formation: $Zr(c) + 0.5Cl_2(g) = ZrCl(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	8.366	60.754	60.754	0	49.100	41.709	-30.573
300	8.372	60.806	60.756	.015	49.096	41.663	-30.351
400	8.612	63.251	61.086	.866	48.892	39.215	-21.426
500	8.761	65.189	61.719	1.735	48.668	36.823	-16.095
600	8.888	66.798	62.436	2.617	48.424	34.475	-12.557
700	9.021	68.178	63.159	3.513	48.167	32.171	-10.044
800	9.162	69.392	63.864	4.422	47.898	29.903	-8.169
900	9.309	70.479	64.540	5.345	47.623	27.671	-6.719
1000	9.453	71.468	65.184	6.284	47.340	25.468	-5.566
1100	9.591	72.375	65.797	7.236	47.049	23.296	-4.628
1136	9.637	72.685	66.010	7.582	46.942	22.520	-4.332
1136	9.637	72.685	66.010	7.582	45.991	22.520	-4.332
1200	9.720	73.215	66.381	8.201	45.891	21.201	-3.861
1300	9.836	73.998	66.937	9.179	45.731	19.149	-3.219
1400	9.940	74.731	67.468	10.168	45.566	17.111	-2.671
1500	10.031	75.420	67.975	11.167	45.393	15.085	-2.198
1600	10.110	76.070	68.461	12.174	45.211	13.069	-1.785
1700	10.178	76.685	68.927	13.189	45.020	11.067	-1.423
1800	10.235	77.268	69.374	14.209	44.818	9.075	-1.102
1900	10.283	77.823	69.805	15.235	44.605	7.094	-.816
2000	10.323	78.351	70.218	16.266	44.379	5.128	-.560

*Data except enthalpy of formation at 298 K estimated.

Phase change: 1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 8.234 + 1.206\times10^{-3}T - 0.202\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 8.234\times10^{-3}T + 0.603\times10^{-6}T^2 + 0.202\times10^{2}T^{-1} - 2.576$

Formation equations (kcal/mol):

298.15-1136 K: $\Delta Hf^\circ = 49.939 - 2.173\times10^{-3}T - 0.383\times10^{-6}T^2 - 46.850T^{-1}$

$\Delta Gf^\circ = 49.939 + 2.173\times10^{-3}T\ln T + 0.383\times10^{-6}T^2 - 23.425T^{-1} - 39.831\times10^{-3}T$

1136-2000 K: $\Delta Hf^\circ = 47.443 - 1.004\times10^{-3}T - 0.252\times10^{-6}T^2 + 7.650T^{-1}$

$\Delta Gf^\circ = 47.443 + 1.004\times10^{-3}T\ln T + 0.252\times10^{-6}T^2 + 3.825T^{-1} - 29.282\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$ZrCl_2(c,l,g)$
Zirconium Dichloride
[Formation: $Zr(c) + Cl_2(g) = ZrCl_2(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	17.350	26.300	26.300	0	-103.000	-92.174	67.565
300	17.378	26.407	26.300	.032	-102.994	-92.107	67.099
400	18.168	31.521	26.991	1.812	-102.684	-88.524	48.367
500	18.700	35.634	28.322	3.656	-102.360	-85.020	37.162
600	19.130	39.082	29.835	5.548	-102.029	-81.584	29.717
700	19.530	42.062	31.375	7.481	-101.687	-78.204	24.416
800	19.868	44.692	32.878	9.451	-101.338	-74.875	20.455
900	20.206	47.052	34.324	11.455	-100.978	-71.587	17.383
1000	20.536	49.199	35.706	13.493	-100.609	-68.342	14.936
1000	21.750	55.599	35.706	19.893	-94.209	-68.342	14.936
1100	21.750	57.672	37.610	22.068	-93.725	-65.778	13.069
1136	21.750	58.372	38.257	22.851	-93.557	-64.867	12.479
1136	21.750	58.372	38.257	22.851	-94.508	-64.867	12.479
1200	21.750	59.564	39.361	24.243	-94.123	-63.206	11.511
1300	21.750	61.305	40.983	26.418	-93.537	-60.655	10.197
1400	21.750	62.917	42.493	28.593	-92.968	-58.146	9.077
1500	21.750	64.418	43.906	30.768	-92.418	-55.679	8.112
1565.3	21.750	65.345	44.782	32.188	-92.069	-54.088	7.552
1565.3	15.119	94.068	44.782	77.148	-47.109	-54.088	7.552
1600	15.146	94.400	45.854	77.673	-47.156	-54.242	7.409
1700	15.232	95.321	48.737	79.192	-47.297	-54.680	7.030
1800	15.323	96.194	51.350	80.720	-47.447	-55.111	6.691
1900	15.419	97.025	53.732	82.257	-47.605	-55.532	6.388
2000	15.516	97.818	55.916	83.804	-47.772	-55.944	6.113

*Data estimated.

Phase changes: 1000 K, melting point of $ZrCl_2$; ΔH° = 6.400 kcal/mol.
1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.
1565.3 K, boiling point of $ZrCl_2$; ΔH° = 44.960 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $Cp^\circ = 17.523 + 3.130\times10^{-3}T - 0.983\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 17.523\times10^{-3}T + 1.565\times10^{-6}T^2 + 0.983\times10^{2}T^{-1} - 5.693$

1000-1565.3 K: $Cp^\circ = 21.750$

$H^\circ - H^\circ_{298} = 21.750\times10^{-3}T - 1.857$

1565.3-2000 K: $Cp^\circ = 13.020 + 1.164\times10^{-3}T + 6.794\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.020\times10^{-3}T + 0.582\times10^{-6}T^2 - 6.794\times10^{2}T^{-1} + 55.776$

$ZrCl_2$(c,l,g) - Continued

Formation equations (kcal/mol):

298.15-1000 K: $\Delta Hf^\circ = -103.844 + 2.703\times10^{-3}T + 0.535\times10^{-6}T^2 - 2.900T^{-1}$

$\Delta Gf^\circ = -103.844 - 2.703\times10^{-3}T\ln T - 0.535\times10^{-6}T^2 - 1.450T^{-1} + 54.716\times10^{-3}T$

1000-1136 K: $\Delta Hf^\circ = -100.007 + 6.930\times10^{-3}T - 1.030\times10^{-6}T^2 - 101.200T^{-1}$

$\Delta Gf^\circ = -100.007 - 6.930\times10^{-3}T\ln T + 1.030\times10^{-6}T^2 - 50.600T^{-1} + 78.563\times10^{-3}T$

1136-1565.3 K: $\Delta Hf^\circ = -102.503 + 8.099\times10^{-3}T - 0.899\times10^{-6}T^2 - 46.700T^{-1}$

$\Delta Gf^\circ = -102.503 - 8.099\times10^{-3}T\ln T + 0.899\times10^{-6}T^2 - 23.350T^{-1} + 89.112\times10^{-3}T$

1565.3-2000 K: $\Delta Hf^\circ = -44.870 - 0.631\times10^{-3}T - 0.317\times10^{-6}T^2 - 726.100T^{-1}$

$\Delta Gf^\circ = -44.870 + 0.631\times10^{-3}T\ln T + 0.317\times10^{-6}T^2 - 363.050T^{-1} - 10.874\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

$ZrCl_2(g)$

Zirconium Dichloride (ideal gas)

[Formation: $Zr(c) + Cl_2(g) = ZrCl_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	13.785	69.896	69.896	0	-44.500	-46.672	34.211
300	13.796	69.981	69.896	.026	-44.500	-46.685	34.009
400	14.231	74.017	70.444	1.429	-44.567	-47.406	25.901
500	14.457	77.219	71.489	2.865	-44.651	-48.104	21.026
600	14.587	79.868	72.671	4.318	-44.759	-48.786	17.770
700	14.668	82.123	73.864	5.781	-44.887	-49.447	15.438
800	14.724	84.085	75.022	7.250	-45.039	-50.090	13.684
900	14.766	85.822	76.128	8.725	-45.208	-50.710	12.314
1000	14.803	87.380	77.176	10.204	-45.398	-51.312	11.214
1100	14.841	88.792	78.168	11.686	-45.607	-51.892	10.310
1136	14.857	89.270	78.513	12.221	-45.687	-52.097	10.023
1136	14.857	89.270	78.513	12.221	-46.638	-52.097	10.023
1200	14.885	90.086	79.109	13.172	-46.694	-52.404	9.544
1300	14.937	91.279	80.000	14.663	-46.792	-52.876	8.889
1400	14.997	92.388	80.845	16.160	-46.901	-53.338	8.326
1500	15.067	93.425	81.650	17.663	-47.023	-53.794	7.838
1600	15.146	94.400	82.417	19.173	-47.156	-54.242	7.409
1700	15.232	95.321	83.149	20.692	-47.297	-54.680	7.030
1800	15.323	96.194	83.850	22.220	-47.447	-55.111	6.691
1900	15.419	97.025	84.521	23.757	-47.605	-55.532	6.388
2000	15.516	97.818	85.166	25.304	-47.772	-55.944	6.113

*Data except enthalpy of formation at 298 K estimated.

Phase change: 1136 K, α - β transition point of Zr; $\Delta H° = 0.951$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 14.607 + 0.324\times10^{-3}T - 0.817\times10^{5}T^{-2}$

$H°- H°_{298} = 14.607\times10^{-3}T + 0.162\times10^{-6}T^2 + 0.817\times10^{2}T^{-1} - 4.644$

Formation equations (kcal/mol):

298.15-1136 K: $\Delta Hf° = -44.294 - 0.213\times10^{-3}T - 0.868\times10^{-6}T^2 - 19.500T^{-1}$

$\Delta Gf° = -44.294 + 0.213\times10^{-3}T\ln T + 0.868\times10^{-6}T^2 - 9.750T^{-1} - 9.340\times10^{-3}T$

1136-2000 K: $\Delta Hf° = -46.790 + 0.956\times10^{-3}T - 0.737\times10^{-6}T^2 + 35.000T^{-1}$

$\Delta Gf° = -46.790 - 0.956\times10^{-3}T\ln T + 0.737\times10^{-6}T^2 + 17.500T^{-1} + 1.209\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$ZrCl_3(c,g)$
Zirconium Trichloride
[Formation: $Zr(c) + 1.5Cl_2(g) = ZrCl_3(c,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	22.990	34.850	34.850	0	-170.700	-154.479	113.235
300	23.019	34.992	34.850	.043	-170.690	-154.378	112.463
400	24.069	41.768	35.768	2.400	-170.219	-149.013	81.416
500	24.730	47.212	37.530	4.841	-169.724	-143.766	62.839
600	25.235	51.767	39.534	7.340	-169.221	-138.623	50.493
700	25.664	55.690	41.567	9.886	-168.704	-133.563	41.700
800	26.064	59.143	43.553	12.472	-168.182	-128.581	35.126
900	26.433	62.234	45.460	15.097	-167.646	-123.660	30.028
1000	26.788	65.038	47.279	17.759	-167.100	-118.803	25.964
1045.9	26.908	66.243	48.085	18.991	-166.848	-116.593	24.363
1045.9	20.709	105.718	48.085	60.278	-125.561	-116.593	24.363
1100	20.756	106.764	50.947	61.399	-125.600	-116.128	23.072
1136	20.778	107.433	52.726	62.147	-125.629	-115.819	22.282
1136	20.778	107.433	52.726	62.147	-126.580	-115.819	22.282
1200	20.817	108.573	55.675	63.478	-126.544	-115.212	20.983
1300	20.860	110.241	59.809	65.562	-126.500	-114.271	19.210
1400	20.889	111.788	63.467	67.650	-126.470	-113.330	17.691
1500	20.907	113.230	66.737	69.740	-126.458	-112.392	16.375
1600	20.915	114.579	69.685	71.831	-126.464	-111.454	15.224
1700	20.917	115.847	72.363	73.923	-126.487	-110.512	14.207
1800	20.913	117.043	74.813	76.014	-126.529	-109.576	13.304
1900	20.906	118.173	77.065	78.105	-126.589	-108.629	12.495
2000	20.895	119.245	79.148	80.195	-126.671	-107.683	11.767

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1045.9 K, sublimation point of $ZrCl_3$; $\Delta H°$ = 41.287 kcal/mol.
1136 K, α - β transition point of Zr; $\Delta H°$ = 0.951 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1045.9 K: $Cp° = 23.692 + 3.246\times10^{-3}T - 1.484\times10^{5}T^{-2}$

$H°- H°_{298} = 23.692\times10^{-3}T + 1.623\times10^{-6}T^2 + 1.484\times10^{2}T^{-1} - 7.706$

1045.9-2000 K: $Cp° = 21.644 - 0.286\times10^{-3}T - 6.951\times10^{5}T^{-2}$

$H°- H°_{298} = 21.644\times10^{-3}T - 0.143\times10^{-6}T^2 + 6.951\times10^{2}T^{-1} + 37.132$

Formation equations (kcal/mol):

298.15-1045.9 K: $\Delta Hf° = -172.122 + 4.458\times10^{-3}T + 0.549\times10^{-6}T^2 + 13.050T^{-1}$

$\Delta Gf° = -172.122 - 4.458\times10^{-3}T\ln T - 0.549\times10^{-6}T^2 + 6.525T^{-1} + 84.667\times10^{-3}T$

1045.9-1136 K: $\Delta Hf° = -127.284 + 2.410\times10^{-3}T - 1.217\times10^{-6}T^2 + 559.750T^{-1}$

$\Delta Gf° = -127.284 - 2.410\times10^{-3}T\ln T + 1.217\times10^{-6}T^2 + 279.875T^{-1} + 25.461\times10^{-3}T$

1136-2000 K: $\Delta Hf° = -129.780 + 3.580\times10^{-3}T - 1.086\times10^{-6}T^2 + 614.250T^{-1}$

$\Delta Gf° = -129.780 - 3.580\times10^{-3}T\ln T + 1.086\times10^{-6}T^2 + 307.125T^{-1} + 36.010\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$ZrCl_3(g)$
Zirconium Trichloride (ideal gas)
[Formation: $Zr(c) + 1.5Cl_2(g) = ZrCl_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	18.170	81.070	81.070	0	-125.300	-122.860	90.057
300	18.189	81.182	81.070	.034	-125.300	-122.844	89.490
400	18.969	86.531	81.793	1.895	-125.324	-122.023	66.669
500	19.487	90.823	83.185	3.819	-125.346	-121.194	52.973
600	19.874	94.412	84.765	5.788	-125.372	-120.362	43.841
700	20.169	97.498	86.368	7.791	-125.400	-119.524	37.317
800	20.389	100.207	87.933	9.819	-125.436	-118.685	32.423
900	20.551	102.618	89.432	11.867	-125.477	-117.836	28.614
1000	20.669	104.790	90.862	13.928	-125.532	-116.986	25.567
1100	20.756	106.764	92.219	15.999	-125.600	-116.128	23.072
1136	20.778	107.433	92.691	16.747	-125.629	-115.819	22.282
1136	20.778	107.433	92.691	16.747	-126.580	-115.819	22.282
1200	20.817	108.573	93.508	18.078	-126.544	-115.212	20.983
1300	20.860	110.241	94.732	20.162	-126.500	-114.271	19.210
1400	20.889	111.788	95.895	22.250	-126.470	-113.330	17.691
1500	20.907	113.230	97.003	24.340	-126.458	-112.392	16.375
1600	20.915	114.579	98.060	26.431	-126.464	-111.454	15.224
1700	20.917	115.847	99.069	28.523	-126.487	-110.512	14.207
1800	20.913	117.043	100.035	30.614	-126.529	-109.576	13.304
1900	20.906	118.173	100.960	32.705	-126.589	-108.629	12.495
2000	20.895	119.245	101.848	34.795	-126.671	-107.683	11.767

*Data except enthalpy of formation at 298 K estimated.

Phase change: 1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.920 + 0.754\times10^{-3}T - 1.755\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.920\times10^{-3}T + 0.377\times10^{-6}T^2 + 1.755\times10^{2}T^{-1} - 6.561$

Formation equations (kcal/mol):

298.15-1136 K: $\Delta Hf^\circ = -125.577 + 0.687\times10^{-3}T - 0.697\times10^{-6}T^2 + 40.150T^{-1}$

$\Delta Gf^\circ = -125.577 - 0.687\times10^{-3}T\ln T + 0.697\times10^{-6}T^2 + 20.075T^{-1} + 12.593\times10^{-3}T$

1136-2000 K: $\Delta Hf^\circ = -128.073 + 1.856\times10^{-3}T - 0.566\times10^{-6}T^2 + 94.650T^{-1}$

$\Delta Gf^\circ = -128.073 - 1.856\times10^{-3}T\ln T + 0.566\times10^{-6}T^2 + 47.325T^{-1} + 23.142\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$ZrCl_4(c,g)$
Zirconium Tetrachloride
[Formation: $Zr(c) + 2Cl_2(g) = ZrCl_4(c,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	28.650	43.400	43.400	0	-234.350	-212.734	155.936
300	28.687	43.577	43.400	.053	-234.338	-212.600	154.877
400	29.952	52.031	44.543	2.995	-233.696	-205.450	112.251
500	30.681	58.795	46.741	6.027	-233.037	-198.464	86.747
600	31.470	64.456	49.234	9.133	-232.361	-191.613	69.794
609.6	31.557	64.954	49.473	9.437	-232.292	-190.958	68.460
609.6	25.190	105.381	49.473	34.081	-207.648	-190.958	68.460
700	25.343	108.875	56.925	36.365	-207.598	-188.488	58.848
800	25.455	112.267	63.634	38.906	-207.564	-185.762	50.747
900	25.533	115.270	69.209	41.455	-207.549	-183.037	44.447
1000	25.589	117.963	73.951	44.012	-207.555	-180.314	39.407
1100	25.631	120.404	78.065	46.573	-207.582	-177.588	35.283
1136	25.643	121.230	79.420	47.496	-207.597	-176.607	33.976
1136	25.643	121.230	79.420	47.496	-208.548	-176.607	33.976
1200	25.663	122.635	81.688	49.137	-208.491	-174.808	31.837
1300	25.688	124.691	84.918	51.705	-208.414	-172.006	28.916
1400	25.708	126.595	87.827	54.275	-208.354	-169.206	26.414
1500	25.724	128.369	90.472	56.846	-208.314	-166.412	24.246
1600	25.737	130.030	92.893	59.419	-208.292	-163.620	22.349
1700	25.748	131.590	95.123	61.994	-208.286	-160.824	20.675
1800	25.757	133.062	97.190	64.569	-208.300	-158.035	19.188
1900	25.765	134.455	99.116	67.145	-208.331	-155.239	17.856
2000	25.771	135.777	100.916	69.722	-208.383	-152.445	16.658

Phase changes: 609.6 K, sublimation point of $ZrCl_4$; $\Delta H° = 24.644$ kcal/mol.
1136 K, α - β transition point of Zr; $\Delta H° = 0.951$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-609.6 K: $Cp° = 29.287 + 4.300\times10^{-3}T - 1.706\times10^{5}T^{-2}$
$H°- H°_{298} = 29.287\times10^{-3}T + 2.150\times10^{-6}T^{2} + 1.706\times10^{2}T^{-1} - 9.495$

609.6-2000 K: $Cp° = 25.804 + 0.016\times10^{-3}T - 2.317\times10^{5}T^{-2}$
$H°- H°_{298} = 25.804\times10^{-3}T + 0.008\times10^{-6}T^{2} + 2.317\times10^{2}T^{-1} + 17.968$

Formation equations (kcal/mol):

298.15-609.6 K: $\Delta Hf° = -236.127 + 5.640\times10^{-3}T + 1.032\times10^{-6}T^{2} + 1.100T^{-1}$
$\Delta Gf° = -236.127 - 5.640\times10^{-3}T\ln T - 1.032\times10^{-6}T^{2} + 0.550T^{-1} + 110.896\times10^{-3}T$

609.6-1136 K: $\Delta Hf° = -208.664 + 2.157\times10^{-3}T - 1.110\times10^{-6}T^{2} + 62.200T^{-1}$
$\Delta Gf° = -208.664 - 2.157\times10^{-3}T\ln T + 1.110\times10^{-6}T^{2} + 31.100T^{-1} + 42.121\times10^{-3}T$

1136-2000 K: $\Delta Hf° = -211.160 + 3.326\times10^{-3}T - 0.979\times10^{-6}T^{2} + 116.700T^{-1}$
$\Delta Gf° = -211.160 - 3.326\times10^{-3}T\ln T + 0.979\times10^{-6}T^{2} + 58.350T^{-1} + 52.671\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (254). Low-temperature heat capacities and entropy at 298 K from Todd (239). High-temperature data for crystal based on Coughlin (39). Data for gas from Chase (26).

$ZrCl_4(g)$
Zirconium Tetrachloride (ideal gas)
[Formation: $Zr(c) + 2Cl_2(g) = ZrCl_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	23.478	87.859	87.859	0	-207.930	-199.570	146.287
300	23.502	88.004	87.861	.043	-207.928	-199.518	145.347
400	24.426	94.908	88.795	2.445	-207.826	-196.731	107.488
500	24.901	100.414	90.586	4.914	-207.730	-193.966	84.781
600	25.174	104.981	92.616	7.419	-207.655	-191.222	69.652
700	25.343	108.875	94.668	9.945	-207.598	-188.488	58.848
800	25.455	112.267	96.660	12.486	-207.564	-185.762	50.747
900	25.533	115.270	98.564	15.035	-207.549	-183.037	44.447
1000	25.589	117.963	100.371	17.592	-207.555	-180.314	39.407
1100	25.631	120.404	102.083	20.153	-207.582	-177.588	35.283
1136	25.643	121.230	102.677	21.076	-207.597	-176.607	33.976
1136	25.643	121.230	102.677	21.076	-208.548	-176.607	33.976
1200	25.663	122.635	103.704	22.717	-208.491	-174.808	31.837
1300	25.688	124.691	105.241	25.285	-208.414	-172.006	28.916
1400	25.708	126.595	106.699	27.855	-208.354	-169.206	26.414
1500	25.724	128.369	108.085	30.426	-208.314	-166.411	24.246
1600	25.737	130.030	109.406	32.999	-208.292	-163.620	22.349
1700	25.748	131.590	110.664	35.574	-208.286	-160.824	20.675
1800	25.757	133.062	111.868	38.149	-208.300	-158.035	19.188
1900	25.765	134.455	113.021	40.725	-208.331	-155.239	17.856
2000	25.771	135.777	114.126	43.302	-208.383	-152.445	16.658

Phase change: 1136 K, α - β transition point of Zr; $\Delta H° = 0.951$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 25.636 + 0.120\times10^{-3}T - 1.950\times10^{5}T^{-2}$

$H°- H°_{298} = 25.636\times10^{-3}T + 0.060\times10^{-6}T^2 + 1.950\times10^{2}T^{-1} - 8.303$

Formation equations (kcal/mol):

298.15-1136 K: $\Delta Hf° = -208.514 + 1.989\times10^{-3}T - 1.058\times10^{-6}T^2 + 25.500T^{-1}$

$\Delta Gf° = -208.514 - 1.989\times10^{-3}T\ln T + 1.058\times10^{-6}T^2 + 12.750T^{-1} + 40.875\times10^{-3}T$

1136-2000 K: $\Delta Hf° = -211.010 + 3.158\times10^{-3}T - 0.927\times10^{-6}T^2 + 80.000T^{-1}$

$\Delta Gf° = -211.010 - 3.158\times10^{-3}T\ln T + 0.927\times10^{-6}T^2 + 40.000T^{-1} + 51.424\times10^{-3}T$

Source: Data from Chase (26).

ZrF(g)

Zirconium Monofluoride (ideal gas)

[Formation: $Zr(c) + 0.5F_2(g) = ZrF(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	7.989	58.227	58.227	0	19.800	12.440	-9.119
300	7.998	58.277	58.227	.015	19.797	12.395	-9.029
400	8.364	60.632	58.547	.834	19.591	9.957	-5.440
500	8.611	62.526	59.158	1.684	19.372	7.575	-3.311
600	8.809	64.114	59.856	2.555	19.136	5.236	-1.907
700	8.993	65.485	60.564	3.445	18.889	2.939	-.918
800	9.176	66.698	61.257	4.353	18.632	.676	-.185
900	9.355	67.789	61.922	5.280	18.369	-1.550	.376
1000	9.528	68.784	62.560	6.224	18.098	-3.750	.820
1100	9.691	69.700	63.168	7.185	17.822	-5.921	1.176
1136	9.745	70.013	63.380	7.535	17.721	-6.697	1.288
1136	9.745	70.013	63.380	7.535	16.770	-6.697	1.288
1200	9.842	70.550	63.748	8.162	16.681	-8.016	1.460
1300	9.979	71.343	64.302	9.153	16.537	-10.069	1.693
1400	10.102	72.087	64.832	10.157	16.389	-12.109	1.890
1500	10.212	72.788	65.339	11.173	16.234	-14.140	2.060
1600	10.309	73.450	65.826	12.199	16.073	-16.159	2.207
1700	10.393	74.078	66.293	13.234	15.903	-18.170	2.336
1800	10.467	74.674	66.742	14.278	15.723	-20.169	2.449
1900	10.531	75.242	67.175	15.328	15.534	-22.158	2.549
2000	10.587	75.783	67.591	16.383	15.331	-24.136	2.637

*Data estimated.

Phase change: 1136 K, α - β transition point of Zr; $\Delta H° = 0.951$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.086 + 1.438\times10^{-3}T - 0.467\times10^{5}T^{-2}$

$H°- H°_{298} = 8.086\times10^{-3}T + 0.719\times10^{-6}T^{2} + 0.467\times10^{2}T^{-1} - 2.631$

Formation equations (kcal/mol):

298.15-1136 K: $\Delta Hf° = 20.594 - 2.161\times10^{-3}T - 0.310\times10^{-6}T^{2} - 36.450T^{-1}$

$\Delta Gf° = 20.594 + 2.161\times10^{-3}T\ln T + 0.310\times10^{-6}T^{2} - 18.225T^{-1} - 39.549\times10^{-3}T$

1136-2000 K: $\Delta Hf° = 18.098 - 0.992\times10^{-3}T - 0.179\times10^{-6}T^{2} + 18.050T^{-1}$

$\Delta Gf° = 18.098 + 0.992\times10^{-3}T\ln T + 0.179\times10^{-6}T^{2} + 9.025T^{-1} - 29.000\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

ZrF_2(c,l)
Zirconium Difluoride
[Formation: $Zr(c) + F_2(g) = ZrF_2(c,l)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	15.760	18.000	18.000	0	-230.000	-218.145	159.902
300	15.780	18.098	18.001	.029	-229.996	-218.071	158.863
400	16.700	22.766	18.631	1.654	-229.780	-214.128	116.993
500	17.500	26.580	19.850	3.365	-229.540	-210.241	91.895
600	18.200	29.834	21.249	5.151	-229.276	-206.407	75.183
700	18.800	32.687	22.684	7.002	-228.986	-202.618	63.260
800	19.270	35.228	24.096	8.906	-228.679	-198.873	54.329
900	19.700	37.523	25.462	10.855	-228.355	-195.165	47.392
1000	20.080	39.619	26.775	12.844	-228.021	-191.497	41.851
1100	20.380	41.547	28.031	14.868	-227.677	-187.859	37.324
1136	20.476	42.205	28.469	15.603	-227.553	-186.559	35.891
1136	20.476	42.205	28.469	15.603	-228.504	-186.559	35.891
1175	20.580	42.898	28.936	16.405	-228.312	-185.120	34.432
1175	24.000	50.558	28.936	25.405	-219.312	-185.120	34.432
1200	24.000	51.063	29.392	26.005	-219.104	-184.395	33.583
1300	24.000	52.984	31.134	28.405	-218.286	-181.536	30.519
1400	24.000	54.763	32.759	30.805	-217.488	-178.740	27.902
1500	24.000	56.419	34.282	33.205	-216.710	-176.000	25.643
1600	24.000	57.968	35.715	35.605	-215.951	-173.311	23.673
1700	24.000	59.423	37.067	38.005	-215.210	-170.668	21.941
1800	24.000	60.795	38.348	40.405	-214.489	-168.071	20.406
1900	24.000	62.092	39.563	42.805	-213.785	-165.510	19.038
2000	24.000	63.323	40.721	45.205	-213.101	-162.987	17.810

*Data estimated.

Phase changes: 1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.
1175 K, melting point of ZrF_2; ΔH° = 9.000 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1175 K: $Cp^\circ = 15.787 + 4.432\times10^{-3}T - 1.199\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 15.787\times10^{-3}T + 2.216\times10^{-6}T^2 + 1.199\times10^{2}T^{-1} - 5.306$

1175-2000 K: $Cp^\circ = 24.000$

$H^\circ - H^\circ_{298} = 24.000\times10^{-3}T - 2.795$

Formation equations (kcal/mol):

298.15-1136 K: $\Delta Hf^\circ = -230.436 + 1.286\times10^{-3}T + 1.100\times10^{-6}T^2 - 13.500T^{-1}$

$\Delta Gf^\circ = -230.436 - 1.286\times10^{-3}T\ln T - 1.100\times10^{-6}T^2 - 6.750T^{-1} + 48.956\times10^{-3}T$

1136-1175 K: $\Delta Hf^\circ = -232.932 + 2.455\times10^{-3}T + 1.231\times10^{-6}T^2 + 41.000T^{-1}$

$\Delta Gf^\circ = -232.932 - 2.455\times10^{-3}T\ln T - 1.231\times10^{-6}T^2 + 20.500T^{-1} + 59.505\times10^{-3}T$

1175-2000 K: $\Delta Hf^\circ = -230.421 + 10.668\times10^{-3}T - 0.985\times10^{-6}T^2 - 78.900T^{-1}$

$\Delta Gf^\circ = -230.421 - 10.668\times10^{-3}T\ln T + 0.985\times10^{-6}T^2 - 39.450T^{-1} + 112.866\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

$ZrF_2(g)$

Zirconium Difluoride (ideal gas)

[Formation: $Zr(c) + F_2(g) = ZrF_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	11.628	67.715	67.715	0	-133.400	-136.367	99.959
300	11.647	67.787	67.715	.022	-133.403	-136.385	99.355
400	12.437	71.257	68.185	1.229	-133.605	-137.350	75.043
500	12.896	74.086	69.090	2.498	-133.807	-138.261	60.433
600	13.176	76.464	70.126	3.803	-134.024	-139.133	50.679
700	13.357	78.509	71.180	5.130	-134.258	-139.966	43.699
800	13.481	80.302	72.212	6.472	-134.513	-140.767	38.455
900	13.572	81.895	73.201	7.825	-134.785	-141.530	34.368
1000	13.646	83.329	74.143	9.186	-135.079	-142.265	31.092
1100	13.711	84.632	75.037	10.554	-135.391	-142.967	28.404
1136	13.734	85.074	75.349	11.048	-135.508	-143.213	27.552
1136	13.734	85.074	75.349	11.048	-136.459	-143.213	27.552
1200	13.776	85.828	75.888	11.928	-136.581	-143.590	26.151
1300	13.844	86.934	76.696	13.309	-136.782	-144.167	24.236
1400	13.918	87.962	77.464	14.697	-136.996	-144.727	22.593
1500	13.999	88.925	78.196	16.093	-137.222	-145.271	21.166
1600	14.086	89.831	78.895	17.497	-137.459	-145.800	19.915
1700	14.180	90.688	79.564	18.910	-137.705	-146.314	18.810
1800	14.277	91.501	80.205	20.333	-137.961	-146.813	17.825
1900	14.378	92.276	80.820	21.766	-138.224	-147.298	16.943
2000	14.479	93.016	81.411	23.209	-138.497	-147.769	16.147

*Data except enthalpy of formation at 298 K estimated.

Phase change: 1136 K, α - β transition point of Zr; $\Delta H° = 0.951$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 13.290 + 0.524\times10^{-3}T - 1.616\times10^{5}T^{-2}$

$H°- H°_{298} = 13.290\times10^{-3}T + 0.262\times10^{-6}T^2 + 1.616\times10^{2}T^{-1} - 4.528$

Formation equations (kcal/mol):

298.15-1136 K: $\Delta Hf° = -133.058 - 1.211\times10^{-3}T - 0.854\times10^{-6}T^2 + 28.200T^{-1}$

$\Delta Gf° = -133.058 + 1.211\times10^{-3}T\ln T + 0.854\times10^{-6}T^2 + 14.100T^{-1} - 18.413\times10^{-3}T$

1136-2000 K: $\Delta Hf° = -135.554 - 0.042\times10^{-3}T - 0.723\times10^{-6}T^2 + 82.700T^{-1}$

$\Delta Gf° = -135.554 + 0.042\times10^{-3}T\ln T + 0.723\times10^{-6}T^2 + 41.350T^{-1} - 7.864\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

$ZrF_3(c)$
Zirconium Trifluoride
[Formation: $Zr(c) + 1.5F_2(g) = ZrF_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	20.000	21.000	21.000	0	-335.000	-316.817	232.230
300	20.150	21.124	21.001	.037	-334.995	-316.705	230.716
400	21.950	27.182	21.814	2.147	-334.678	-310.653	169.731
500	23.150	32.215	23.405	4.405	-334.293	-304.689	133.178
600	24.000	36.515	25.240	6.765	-333.870	-298.809	108.840
700	24.600	40.261	27.125	9.195	-333.426	-293.001	91.478
800	25.100	43.580	28.978	11.682	-332.966	-287.258	78.474
900	25.450	46.557	30.768	14.210	-332.499	-281.569	68.374
1000	25.750	49.225	32.454	16.771	-332.033	-275.907	60.299
1100	25.930	51.719	34.124	19.355	-331.572	-270.350	53.713
1136	25.962	52.555	34.694	20.289	-331.409	-268.350	51.626
1136	25.962	52.555	34.694	20.289	-332.360	-268.350	51.626
1200	26.020	53.979	35.685	21.953	-331.983	-264.753	48.217
1300	26.100	56.065	37.173	24.559	-331.407	-259.174	43.571
1400	26.170	58.001	38.592	27.173	-330.845	-253.638	39.594
1500	26.230	59.809	39.947	29.793	-330.298	-248.143	36.154

*Data estimated.

Phase change: 1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $Cp^\circ = 23.603 + 2.324\times10^{-3}T - 3.818\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 23.603\times10^{-3}T + 1.162\times10^{-6}T^2 + 3.818\times10^{2}T^{-1} - 8.421$

Formation equations (kcal/mol):

298.15-1136 K: $\Delta Hf^\circ = -337.106 + 4.848\times10^{-3}T - 0.041\times10^{-6}T^2 + 198.150T^{-1}$

$\Delta Gf^\circ = -337.106 - 4.848\times10^{-3}T\ln T + 0.041\times10^{-6}T^2 + 99.075T^{-1} + 94.545\times10^{-3}T$

1136-1500 K: $\Delta Hf^\circ = -339.602 + 6.017\times10^{-3}T + 0.090\times10^{-6}T^2 + 252.650T^{-1}$

$\Delta Gf^\circ = -339.602 - 6.017\times10^{-3}T\ln T - 0.090\times10^{-6}T^2 + 126.325T^{-1} + 105.094\times10^{-3}T$

Source: Data are those estimated by JANAF (60).

$ZrF_3(g)$
Zirconium Trifluoride (ideal gas)
[Formation: $Zr(c) + 1.5F_2(g) = ZrF_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	16.212	73.047	73.047	0	-264.200	-261.535	191.708
300	16.244	73.147	73.047	.030	-264.202	-261.519	190.514
400	17.616	78.023	73.703	1.728	-264.298	-260.609	142.388
500	18.524	82.058	74.982	3.538	-264.361	-259.678	113.504
600	19.165	85.495	76.455	5.424	-264.411	-258.738	94.244
700	19.628	88.486	77.965	7.365	-264.456	-257.788	80.484
800	19.965	91.130	79.447	9.346	-264.503	-256.834	70.163
900	20.210	93.496	80.879	11.355	-264.554	-255.869	62.133
1000	20.390	95.636	82.250	13.386	-264.618	-254.904	55.708
1100	20.523	97.586	83.557	15.432	-264.695	-253.927	50.450
1136	20.558	98.247	84.012	16.171	-264.727	-253.575	48.783
1136	20.558	98.247	84.012	16.171	-265.678	-253.575	48.783
1200	20.620	99.376	84.802	17.489	-265.648	-252.893	46.058
1300	20.692	101.029	85.987	19.555	-265.611	-251.831	42.336
1400	20.743	102.565	87.117	21.627	-265.591	-250.773	39.147
1500	20.779	103.997	88.195	23.703	-265.589	-249.715	36.383
1600	20.803	105.339	89.225	25.782	-265.604	-248.656	33.964
1700	20.817	106.601	90.211	27.863	-265.635	-247.596	31.830
1800	20.824	107.791	91.155	29.945	-265.689	-246.535	29.933
1900	20.825	108.917	92.060	32.028	-265.758	-245.468	28.235
2000	20.822	109.985	92.930	34.110	-265.851	-244.399	26.706

*Data except enthalpy of formation at 298 K estimated.

Phase change: 1136 K, α - β transition point of Zr; $\Delta H° = 0.951$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 19.356 + 1.104\times10^{-3}T - 3.088\times10^{5}T^{-2}$

$H°- H°_{298} = 19.356\times10^{-3}T + 0.552\times10^{-6}T^2 + 3.088\times10^{2}T^{-1} - 6.856$

Formation equations (kcal/mol):

298.15-1136 K: $\Delta Hf° = -264.741 + 0.601\times10^{-3}T - 0.651\times10^{-6}T^2 + 125.150T^{-1}$

$\Delta Gf° = -264.741 - 0.601\times10^{-3}T\ln T + 0.651\times10^{-6}T^2 + 62.575T^{-1} + 13.279\times10^{-3}T$

1136-2000 K: $\Delta Hf° = -267.237 + 1.770\times10^{-3}T - 0.520\times10^{-6}T^2 + 179.650T^{-1}$

$\Delta Gf° = -267.237 - 1.770\times10^{-3}T\ln T + 0.520\times10^{-6}T^2 + 89.825T^{-1} + 23.828\times10^{-3}T$

Source: Data from JANAF (60) who estimated all except enthalpy of formation at 298 K.

ZrF_4(c,g)
Zirconium Tetrafluoride
[Formation: $Zr(c) + 2F_2(g) = ZrF_4(c,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	24.790	25.000	25.000	0	-456.800	-432.588	317.092
300	24.853	25.154	25.001	.046	-456.793	-432.438	315.027
400	27.237	32.670	26.010	2.664	-456.353	-424.383	231.869
500	28.586	38.904	27.984	5.460	-455.832	-416.449	182.027
600	29.529	44.203	30.256	8.368	-455.276	-408.625	148.840
700	30.281	48.813	32.584	11.360	-454.693	-400.895	125.164
800	30.931	52.900	34.874	14.421	-454.091	-393.253	107.430
900	31.522	56.577	37.084	17.544	-453.464	-385.682	93.655
1000	32.075	59.928	39.204	20.724	-452.819	-378.189	82.652
1100	32.605	63.010	41.229	23.959	-452.150	-370.755	73.661
1136	32.790	64.063	41.936	25.136	-451.904	-368.096	70.815
1136	32.790	64.063	41.936	25.136	-452.855	-368.096	70.815
1179	33.012	65.285	42.766	26.550	-452.497	-364.895	67.639
1179	25.374	109.081	42.766	78.185	-400.862	-364.895	67.639
1200	25.391	109.529	43.931	78.718	-400.846	-364.254	66.339
1300	25.455	111.564	49.056	81.260	-400.781	-361.208	60.724
1400	25.506	113.453	53.590	83.808	-400.735	-358.168	55.912
1500	25.548	115.214	57.640	86.361	-400.707	-355.128	51.741
1600	25.582	116.864	61.290	88.918	-400.697	-352.089	48.093
1700	25.610	118.415	64.605	91.477	-400.705	-349.049	44.873
1800	25.634	119.880	67.636	94.039	-400.734	-346.012	42.011
1900	25.654	121.266	70.422	96.604	-400.778	-342.969	39.450
2000	25.671	122.583	72.998	99.170	-400.845	-339.927	37.145

Phase changes: 1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.
1179 K, sublimation point of ZrF_4; ΔH° = 51.635 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1179 K: $Cp^\circ = 27.864 + 4.606\times10^{-3}T - 3.953\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 27.864\times10^{-3}T + 2.303\times10^{-6}T^2 + 3.953\times10^{2}T^{-1} - 9.838$

1179-2000 K: $Cp^\circ = 25.786 + 0.020\times10^{-3}T - 6.054\times10^{5}T^{-2}$
$H^\circ - H^\circ_{298} = 25.786\times10^{-3}T + 0.010\times10^{-6}T^2 + 6.054\times10^{2}T^{-1} + 47.256$

Formation equations (kcal/mol):

298.15-1136 K: $\Delta Hf^\circ = -458.879 + 4.855\times10^{-3}T + 1.013\times10^{-6}T^2 + 161.400T^{-1}$
$\Delta Gf^\circ = -458.879 - 4.855\times10^{-3}T\ln T - 1.013\times10^{-6}T^2 + 80.700T^{-1} + 115.235\times10^{-3}T$

1136-1179 K: $\Delta Hf^\circ = -461.375 + 6.024\times10^{-3}T + 1.144\times10^{-6}T^2 + 215.900T^{-1}$
$\Delta Gf^\circ = -461.375 - 6.024\times10^{-3}T\ln T - 1.144\times10^{-6}T^2 + 107.950T^{-1} + 125.784\times10^{-3}T$

1179-2000 K: $\Delta Hf^\circ = -404.281 + 3.946\times10^{-3}T - 1.149\times10^{-6}T^2 + 426.000T^{-1}$
$\Delta Gf^\circ = -404.281 - 3.946\times10^{-3}T\ln T + 1.149\times10^{-6}T^2 + 213.000T^{-1} + 59.882\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (254). Low-temperature heat capacities and entropy at 298 K from Westrum (260). High-temperature data for crystal based on McDonald (158). Gas data from Chase (26).

$ZrF_4(g)$

Zirconium Tetrafluoride (ideal gas)

[Formation: $Zr(c) + 2F_2(g) = ZrF_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15	20.887	76.339	76.339	0	-400.000	-391.095	286.677
300	20.927	76.468	76.339	.039	-400.000	-391.040	284.868
400	22.603	82.740	77.182	2.223	-399.994	-388.052	212.019
500	23.593	87.899	78.825	4.537	-399.955	-385.070	168.312
600	24.205	92.259	80.711	6.929	-399.915	-382.098	139.177
700	24.603	96.022	82.635	9.371	-399.882	-379.130	118.368
800	24.873	99.326	84.520	11.845	-399.867	-376.170	102.764
900	25.065	102.267	86.330	14.343	-399.865	-373.204	90.625
1000	25.205	104.916	88.060	16.856	-399.887	-370.245	80.916
1100	25.310	107.323	89.703	19.382	-399.927	-367.277	72.970
1136	25.339	108.139	90.274	20.294	-399.947	-366.208	70.452
1136	25.339	108.139	90.274	20.294	-400.898	-366.208	70.452
1200	25.391	109.529	91.264	21.918	-400.846	-364.254	66.339
1300	25.455	111.564	92.749	24.460	-400.781	-361.208	60.724
1400	25.506	113.453	94.162	27.008	-400.735	-358.168	55.912
1500	25.548	115.214	95.507	29.561	-400.707	-355.128	51.741
1600	25.582	116.864	96.790	32.118	-400.697	-352.089	48.093
1700	25.610	118.415	98.017	34.677	-400.705	-349.049	44.873
1800	25.634	119.880	99.192	37.239	-400.734	-346.012	42.011
1900	25.654	121.266	100.317	39.804	-400.778	-342.969	39.450
2000	25.671	122.583	101.398	42.370	-400.845	-339.927	37.145

Phase change: 1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 24.920 + 0.534\times10^{-3}T - 3.726\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 24.920\times10^{-3}T + 0.267\times10^{-6}T^2 + 3.726\times10^{2}T^{-1} - 8.703$

Formation equations (kcal/mol):

298.15-1136 K: $\Delta Hf^\circ = -400.944 + 1.911\times10^{-3}T - 1.023\times10^{-6}T^2 + 138.700T^{-1}$

$\Delta Gf^\circ = -400.944 - 1.911\times10^{-3}T\ln T + 1.023\times10^{-6}T^2 + 69.350T^{-1} + 42.836\times10^{-3}T$

1136-2000 K: $\Delta Hf^\circ = -403.440 + 3.080\times10^{-3}T - 0.892\times10^{-6}T^2 + 193.200T^{-1}$

$\Delta Gf^\circ = -403.440 - 3.080\times10^{-3}T\ln T + 0.892\times10^{-6}T^2 + 96.600T^{-1} + 53.385\times10^{-3}T$

Source: Data from Chase (26) who estimated some molecular constants.

ZrI(g)

Zirconium Monoiodide (ideal gas)

[Formation: $Zr(c) + 0.5I_2(c,l,g) = ZrI(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15*	8.823	65.868	65.868	0	96.300	83.578	-61.264
300	8.825	65.923	65.870	.016	96.293	83.499	-60.828
386.8	8.911	68.178	66.145	.786	95.905	79.846	-45.114
386.8	8.911	68.178	66.145	.786	94.051	79.846	-45.114
400	8.924	68.477	66.217	.904	93.955	79.363	-43.361
458.4	8.958	69.696	66.583	1.427	93.529	77.264	-36.836
458.4	8.958	69.696	66.583	1.427	88.519	77.264	-36.836
500	8.983	70.475	66.875	1.800	88.425	76.248	-33.327
600	9.025	72.116	67.616	2.700	88.185	73.833	-26.893
700	9.059	73.510	68.360	3.605	87.927	71.463	-22.311
800	9.089	74.722	69.082	4.512	87.649	69.128	-18.885
900	9.116	75.794	69.770	5.422	87.353	66.831	-16.229
1000	9.142	76.756	70.421	6.335	87.038	64.568	-14.111
1100	9.166	77.628	71.036	7.251	86.707	62.338	-12.385
1136	9.175	77.923	71.250	7.581	86.582	61.542	-11.840
1136	9.175	77.923	71.250	7.581	85.631	61.542	-11.840
1200	9.190	78.427	71.620	8.168	85.496	60.188	-10.962
1300	9.214	79.163	72.171	9.089	85.275	58.089	-9.765
1400	9.237	79.847	72.696	10.011	85.040	56.006	-8.743
1500	9.259	80.485	73.194	10.936	84.789	53.941	-7.859
1600	9.282	81.083	73.669	11.863	84.524	51.894	-7.088
1700	9.304	81.647	74.122	12.792	84.244	49.861	-6.410
1800	9.327	82.179	74.555	13.724	83.951	47.847	-5.809
1900	9.349	82.684	74.969	14.658	83.642	45.849	-5.274
2000	9.371	83.164	75.367	15.594	83.319	43.869	-4.794

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; $\Delta H°$ = 3.709 kcal/mol.
458.4 K, boiling point of I_2; $\Delta H°$ = 10.021 kcal/mol.
1136 K, α - β transition point of Zr; $\Delta H°$ = 0.951 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 8.935 + 0.222\times10^{-3}T - 0.159\times10^{5}T^{-2}$

$H°- H°_{298} = 8.935\times10^{-3}T + 0.111\times10^{-6}T^{2} + 0.159\times10^{2}T^{-1} - 2.727$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = 97.540 - 3.496\times10^{-3}T - 1.577\times10^{-6}T^{2} - 17.000T^{-1}$

$\Delta Gf° = 97.540 + 3.496\times10^{-3}T\ln T + 1.577\times10^{-6}T^{2} - 8.500T^{-1} - 67.123\times10^{-3}T$

386.8-458.4 K: $\Delta Hf° = 96.812 - 6.699\times10^{-3}T - 0.831\times10^{-6}T^{2} - 17.000T^{-1}$

$\Delta Gf° = 96.812 + 6.699\times10^{-3}T\ln T + 0.831\times10^{-6}T^{2} - 8.500T^{-1} - 84.031\times10^{-3}T$

458.4-1136 K: $\Delta Hf° = 89.456 - 1.528\times10^{-3}T - 0.865\times10^{-6}T^{2} - 24.650T^{-1}$

$\Delta Gf° = 89.456 + 1.528\times10^{-3}T\ln T + 0.865\times10^{-6}T^{2} - 12.325T^{-1} - 36.299\times10^{-3}T$

1136-2000 K: $\Delta Hf° = 86.960 - 0.359\times10^{-3}T - 0.734\times10^{-6}T^{2} + 29.850T^{-1}$

$\Delta Gf° = 86.960 + 0.359\times10^{-3}T\ln T + 0.734\times10^{-6}T^{2} + 14.925T^{-1} - 25.750\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Kleinschmidt (131). Other data are those estimated by JANAF (60).

ZrI_2(c,l,g)
Zirconium Diiodide
[Formation: $Zr(c) + I_2(c,l,g) = ZrI_2(c,l,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	22.500	35.900	35.900	0	-66.400	-66.049	48.414
300	22.550	36.039	35.900	.042	-66.393	-66.046	48.114
386.8	22.689	41.906	36.616	2.046	-66.151	-65.982	37.281
386.8	22.689	41.906	36.616	2.046	-69.860	-65.982	37.281
400	22.710	42.668	36.803	2.346	-69.901	-65.849	35.978
458.4	22.827	45.771	37.752	3.676	-70.083	-65.242	31.105
458.4	22.827	45.771	37.752	3.676	-80.104	-65.242	31.105
500	22.910	47.757	38.503	4.627	-79.805	-63.905	27.932
600	23.090	51.951	40.404	6.928	-79.093	-60.793	22.144
700	23.290	55.525	42.314	9.247	-78.386	-57.797	18.045
700	23.290	64.095	42.314	15.247	-72.386	-57.797	18.045
800	25.370	67.320	45.241	17.663	-71.606	-55.766	15.234
900	27.460	70.429	47.868	20.305	-70.622	-53.842	13.075
1000	29.540	73.429	50.274	23.155	-69.452	-52.038	11.373
1100	31.620	76.342	52.512	26.213	-68.095	-50.361	10.006
1136	32.369	77.372	53.284	27.365	-67.561	-49.790	9.579
1136	32.369	77.372	53.284	27.365	-68.512	-49.790	9.579
1200	33.700	79.183	54.617	29.479	-67.411	-48.764	8.881
1295.3	35.680	81.834	56.523	32.785	-65.626	-47.353	7.990
1295.3	13.898	102.703	56.523	59.817	-38.594	-47.353	7.990
1300	13.898	102.753	56.690	59.882	-38.604	-47.384	7.966
1400	13.900	103.783	60.017	61.272	-38.828	-48.050	7.501
1500	13.901	104.742	62.967	62.662	-39.070	-48.701	7.096
1600	13.903	105.639	65.606	64.053	-39.328	-49.333	6.738
1700	13.903	106.482	67.986	65.443	-39.605	-49.951	6.422
1800	13.904	107.277	70.148	66.833	-39.899	-50.553	6.138
1900	13.905	108.028	72.121	68.224	-40.210	-51.135	5.882
2000	13.906	108.742	73.935	69.614	-40.539	-51.703	5.650

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
700 K, melting point of ZrI_2; ΔH° = 6.000 kcal/mol.
1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.
1295.3 K, boiling point of ZrI_2; ΔH° = 27.032 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $Cp^\circ = 24.411 - 1.574\times10^{-3}T - 1.281\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 24.411\times10^{-3}T - 0.787\times10^{-6}T^2 + 1.281\times10^{2}T^{-1} - 7.638$

700-1295.30 K: $Cp^\circ = 7.569 + 21.628\times10^{-3}T + 2.848\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 7.569\times10^{-3}T + 10.814\times10^{-6}T^2 - 2.848\times10^{2}T^{-1} + 5.057$

1295.3-2000 K: $Cp^\circ = 13.641 + 0.122\times10^{-3}T + 1.679\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.641\times10^{-3}T + 0.061\times10^{-6}T^2 - 1.679\times10^{2}T^{-1} + 42.175$

ZrI_2(c,l,g) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -68.085 + 5.541\times10^{-3}T - 3.221\times10^{-6}T^2 + 95.200T^{-1}$

$\Delta Gf^\circ = -68.085 - 5.541\times10^{-3}T\ln T + 3.221\times10^{-6}T^2 + 47.600T^{-1} + 36.904\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -69.540 - 0.863\times10^{-3}T - 1.729\times10^{-6}T^2 + 95.200T^{-1}$

$\Delta Gf^\circ = -69.540 + 0.863\times10^{-3}T\ln T + 1.729\times10^{-6}T^2 + 47.600T^{-1} + 3.089\times10^{-3}T$

458.4-700 K: $\Delta Hf^\circ = -84.253 + 9.477\times10^{-3}T - 1.797\times10^{-6}T^2 + 79.900T^{-1}$

$\Delta Gf^\circ = -84.253 - 9.477\times10^{-3}T\ln T + 1.797\times10^{-6}T^2 + 39.950T^{-1} + 98.552\times10^{-3}T$

700-1136 K: $\Delta Hf^\circ = -71.559 - 7.365\times10^{-3}T + 9.804\times10^{-6}T^2 - 333.000T^{-1}$

$\Delta Gf^\circ = -71.559 + 7.365\times10^{-3}T\ln T - 9.804\times10^{-6}T^2 - 166.500T^{-1} - 21.375\times10^{-3}T$

1136-1295.3 K: $\Delta Hf^\circ = -74.055 - 6.196\times10^{-3}T + 9.935\times10^{-6}T^2 - 278.500T^{-1}$

$\Delta Gf^\circ = -74.055 + 6.196\times10^{-3}T\ln T - 9.935\times10^{-6}T^2 - 139.250T^{-1} - 10.826\times10^{-3}T$

1295.3-2000 K: $\Delta Hf^\circ = -36.937 - 0.124\times10^{-3}T - 0.818\times10^{-6}T^2 - 161.600T^{-1}$

$\Delta Gf^\circ = -36.937 + 0.124\times10^{-3}T\ln T + 0.818\times10^{-6}T^2 - 80.800T^{-1} - 9.930\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Lamoreaux (138). Other data are those estimated by JANAF (60).

$ZrI_2(g)$

Zirconium Diiodide (ideal gas)

[Formation: $Zr(c) + I_2(c,l,g) = ZrI_2(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	13.681	82.380	82.380	0	-20.400	-33.907	24.854
300	13.683	82.465	82.382	.025	-20.410	-33.990	24.762
386.8	13.768	85.954	82.807	1.217	-20.980	-37.849	21.385
386.8	13.768	85.954	82.807	1.217	-24.689	-37.849	21.385
400	13.781	86.416	82.919	1.399	-24.848	-38.296	20.923
458.4	13.808	88.297	83.486	2.205	-25.553	-40.207	19.169
458.4	13.808	88.297	83.486	2.205	-35.574	-40.207	19.169
500	13.827	89.497	83.937	2.780	-35.652	-40.622	17.756
600	13.852	92.020	85.080	4.164	-35.857	-41.598	15.152
700	13.868	94.157	86.228	5.550	-36.083	-42.538	13.281
800	13.878	96.009	87.338	6.937	-36.332	-43.443	11.868
900	13.885	97.644	88.394	8.325	-36.602	-44.316	10.761
1000	13.890	99.107	89.393	9.714	-36.893	-45.157	9.869
1100	13.893	100.431	90.337	11.103	-37.205	-45.969	9.133
1136	13.894	100.878	90.664	11.603	-37.323	-46.254	8.898
1136	13.894	100.878	90.664	11.603	-38.274	-46.254	8.898
1200	13.896	101.640	91.229	12.493	-38.397	-46.699	8.505
1300	13.898	102.753	92.075	13.882	-38.604	-47.384	7.966
1400	13.900	103.783	92.874	15.272	-38.828	-48.050	7.501
1500	13.901	104.742	93.634	16.662	-39.070	-48.701	7.096
1600	13.903	105.639	94.356	18.053	-39.328	-49.333	6.738
1700	13.903	106.482	95.045	19.443	-39.605	-49.951	6.422
1800	13.904	107.277	95.703	20.833	-39.899	-50.553	6.138
1900	13.905	108.028	96.331	22.224	-40.210	-51.135	5.882
2000	13.906	108.742	96.935	23.614	-40.539	-51.703	5.650

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 13.904 + 0.004\times10^{-3}T - 0.199\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 13.904\times10^{-3}T + 0.002\times10^{-6}T^2 + 0.199\times10^{2}T^{-1} - 4.212$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -18.660 - 4.966\times10^{-3}T - 2.432\times10^{-6}T^2 - 13.000T^{-1}$

$\Delta Gf^\circ = -18.660 + 4.966\times10^{-3}T\ln T + 2.432\times10^{-6}T^2 - 6.500T^{-1} - 80.086\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -20.115 - 11.370\times10^{-3}T - 0.940\times10^{-6}T^2 - 13.000T^{-1}$

$\Delta Gf^\circ = -20.115 + 11.370\times10^{-3}T\ln T + 0.940\times10^{-6}T^2 - 6.500T^{-1} - 113.901\times10^{-3}T$

458.4-1136 K: $\Delta Hf^\circ = -34.828 - 1.030\times10^{-3}T - 1.008\times10^{-6}T^2 - 28.300T^{-1}$

$\Delta Gf^\circ = -34.828 + 1.030\times10^{-3}T\ln T + 1.008\times10^{-6}T^2 - 14.150T^{-1} - 18.438\times10^{-3}T$

1136-2000 K: $\Delta Hf^\circ = -37.324 + 0.139\times10^{-3}T - 0.877\times10^{-6}T^2 + 26.200T^{-1}$

$\Delta Gf^\circ = -37.324 - 0.139\times10^{-3}T\ln T + 0.877\times10^{-6}T^2 + 13.100T^{-1} - 7.889\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Lamoreaux (138) and JANAF (60). Other data are those estimated by JANAF (60).

$ZrI_3(c)$

Zirconium Triiodide

[Formation: $Zr(c) + 1.5I_2(c,l,g) = ZrI_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	24.813	48.897	48.897	0	-93.600	-92.986	68.160
300	24.832	49.051	48.898	.046	-93.601	-92.981	67.736
386.8	25.238	55.419	49.673	2.222	-93.790	-92.783	52.424
386.8	25.238	55.419	49.673	2.222	-99.354	-92.783	52.424
400	25.300	56.267	49.877	2.556	-99.489	-92.557	50.570
458.4	25.358	59.718	50.916	4.035	-100.084	-91.499	43.623
458.4	25.358	59.718	50.916	4.035	-115.115	-91.499	43.623
500	25.400	61.923	51.741	5.091	-114.898	-89.363	39.060
600	25.500	66.564	53.837	7.636	-114.390	-84.306	30.708
700	25.550	70.499	55.943	10.189	-113.899	-79.331	24.768
800	25.600	73.914	57.982	12.746	-113.428	-74.425	20.332
900	25.650	76.932	59.922	15.309	-112.976	-69.576	16.895

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-900 K: $Cp^\circ = 25.905 - 0.216\times10^{-3}T - 0.913\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.905\times10^{-3}T - 0.108\times10^{-6}T^2 + 0.913\times10^{2}T^{-1} - 8.020$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -93.681 + 0.596\times10^{-3}T - 3.288\times10^{-6}T^2 + 58.400T^{-1}$

$\Delta Gf^\circ = -93.681 - 0.596\times10^{-3}T\ln T + 3.288\times10^{-6}T^2 + 29.200T^{-1} + 4.423\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -95.864 - 9.010\times10^{-3}T - 1.050\times10^{-6}T^2 + 58.400T^{-1}$

$\Delta Gf^\circ = -95.864 + 9.010\times10^{-3}T\ln T + 1.050\times10^{-6}T^2 + 29.200T^{-1} - 46.300\times10^{-3}T$

458.4-900 K: $\Delta Hf^\circ = -117.934 + 6.500\times10^{-3}T - 1.152\times10^{-6}T^2 + 35.450T^{-1}$

$\Delta Gf^\circ = -117.934 - 6.500\times10^{-3}T\ln T + 1.152\times10^{-6}T^2 + 17.725T^{-1} + 96.894\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Lamoreaux (138). Other data are those estimated by JANAF (60).

$ZrI_3(g)$

Zirconium Triiodide (ideal gas)

[Formation: $Zr(c) + 1.5I_2(c,l,g) = ZrI_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	19.317	95.047	95.047	0	-30.800	-43.945	32.212
300	19.324	95.166	95.047	.036	-30.811	-44.026	32.072
386.8	19.526	100.106	95.652	1.723	-31.490	-47.767	26.989
386.8	19.526	100.106	95.652	1.723	-37.053	-47.767	26.989
400	19.557	100.762	95.810	1.981	-37.264	-48.130	26.296
458.4	19.622	103.432	96.614	3.126	-38.193	-49.647	23.670
458.4	19.622	103.432	96.614	3.126	-53.225	-49.647	23.670
500	19.669	105.139	97.253	3.943	-53.246	-49.319	21.557
600	19.730	108.731	98.874	5.914	-53.313	-48.528	17.676
700	19.768	111.776	100.506	7.889	-53.399	-47.724	14.900
800	19.792	114.417	102.083	9.867	-53.507	-46.906	12.814
900	19.809	116.749	103.586	11.847	-53.638	-46.073	11.188
1000	19.821	118.837	105.009	13.828	-53.789	-45.225	9.884
1100	19.830	120.727	106.353	15.811	-53.961	-44.361	8.814
1136	19.833	121.366	106.819	16.525	-54.028	-44.047	8.474
1136	19.833	121.366	106.819	16.525	-54.979	-44.047	8.474
1200	19.837	122.452	107.624	17.794	-55.014	-43.428	7.909
1300	19.842	124.040	108.826	19.778	-55.080	-42.460	7.138
1400	19.846	125.511	109.966	21.763	-55.166	-41.485	6.476
1500	19.850	126.880	111.049	23.747	-55.270	-40.506	5.902
1600	19.852	128.161	112.078	25.733	-55.390	-39.515	5.397
1700	19.855	129.365	113.060	27.718	-55.530	-38.521	4.952
1800	19.857	130.500	113.998	29.703	-55.688	-37.517	4.555
1900	19.858	131.574	114.896	31.689	-55.863	-36.504	4.199
2000	19.860	132.592	115.754	33.675	-56.056	-35.478	3.877

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp^\circ = 19.862 + 0.006\times10^{-3}T - 0.486\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 19.862\times10^{-3}T + 0.003\times10^{-6}T^2 + 0.486\times10^{2}T^{-1} - 6.085$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -28.946 - 5.447\times10^{-3}T - 3.177\times10^{-6}T^2 + 15.700T^{-1}$

$\Delta Gf^\circ = -28.946 + 5.447\times10^{-3}T\ln T + 3.177\times10^{-6}T^2 + 7.850T^{-1} - 82.375\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -31.129 - 15.053\times10^{-3}T - 0.939\times10^{-6}T^2 + 15.700T^{-1}$

$\Delta Gf^\circ = -31.129 + 15.053\times10^{-3}T\ln T + 0.939\times10^{-6}T^2 + 7.850T^{-1} - 133.098\times10^{-3}T$

458.4-1136 K: $\Delta Hf^\circ = -53.199 + 0.457\times10^{-3}T - 1.041\times10^{-6}T^2 - 7.250T^{-1}$

$\Delta Gf^\circ = -53.199 - 0.457\times10^{-3}T\ln T + 1.041\times10^{-6}T^2 - 3.625T^{-1} + 10.097\times10^{-3}T$

1136-2000 K: $\Delta Hf^\circ = -55.695 + 1.627\times10^{-3}T - 0.910\times10^{-6}T^2 + 47.250T^{-1}$

$\Delta Gf^\circ = -55.695 - 1.627\times10^{-3}T\ln T + 0.910\times10^{-6}T^2 + 23.625T^{-1} + 20.646\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Kleinschmidt (131). Other data are those estimated by JANAF (60).

$ZrI_4(c,g)$

Zirconium Tetraiodide

[Formation: $Zr(c) + 2I_2(c,l,g) = ZrI_4(c,g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H^\circ_{298})/T$	$H^\circ - H^\circ_{298}$	ΔHf°	ΔGf°	
298.15*	29.900	59.800	59.800	0	-116.800	-115.299	84.515
300	29.916	59.985	59.802	.055	-116.804	-115.289	83.987
386.8	30.536	67.674	60.737	2.683	-117.146	-114.812	64.870
386.8	30.536	67.674	60.737	2.683	-124.564	-114.812	64.870
400	30.630	68.700	60.982	3.087	-124.756	-114.476	62.546
458.4	30.940	72.893	62.235	4.885	-125.594	-112.910	53.831
458.4	30.940	72.893	62.235	4.885	-145.636	-112.910	53.831
500	31.160	75.590	63.236	6.177	-145.369	-109.949	48.058
600	31.610	81.320	65.793	9.316	-144.716	-102.933	37.493
700	32.040	86.220	68.363	12.500	-144.043	-96.017	29.977
702.6	32.050	86.340	68.431	12.583	-144.026	-95.840	29.811
702.6	25.674	128.495	68.431	42.201	-114.408	-95.840	29.811
800	25.710	131.831	75.952	44.703	-114.377	-93.268	25.479
900	25.736	134.861	82.333	47.275	-114.367	-90.631	22.008
1000	25.754	137.573	87.723	49.850	-114.377	-87.992	19.230
1100	25.768	140.029	92.369	52.426	-114.409	-85.354	16.958
1136	25.772	140.859	93.893	53.354	-114.426	-84.403	16.238
1136	25.772	140.859	93.893	53.354	-115.377	-84.403	16.238
1200	25.778	142.271	96.435	55.003	-115.323	-82.658	15.054
1300	25.786	144.335	100.041	57.582	-115.249	-79.938	13.439
1400	25.793	146.246	103.274	60.161	-115.196	-77.222	12.055
1500	25.798	148.026	106.199	62.740	-115.162	-74.515	10.857
1600	25.802	149.691	108.866	65.320	-115.145	-71.803	9.808
1700	25.806	151.255	111.313	67.901	-115.147	-69.094	8.883
1800	25.809	152.731	113.575	70.481	-115.168	-66.388	8.061
1900	25.811	154.126	115.672	73.062	-115.208	-63.676	7.324
2000	25.813	155.450	117.628	75.644	-115.265	-60.961	6.661

*Heat capacity at 298 K estimated.

Phase changes: 386.8 K, melting point of I_2; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I_2; ΔH° = 10.021 kcal/mol.
702.6 K, sublimation point of ZrI_4; ΔH° = 29.618 kcal/mol.
1136 K, α - β transition point of Zr; ΔH° = 0.951 kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-702.6 K: $Cp^\circ = 29.660 + 3.610\times10^{-3}T - 0.743\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 29.660\times10^{-3}T + 1.805\times10^{-6}T^2 + 0.743\times10^{2}T^{-1} - 9.253$

702.6-2000 K: $Cp^\circ = 25.834 - 0.785\times10^{5}T^{-2}$

$H^\circ - H^\circ_{298} = 25.834\times10^{-3}T + 0.785\times10^{2}T^{-1} + 23.938$

ZrI_4(c,g) - Continued

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf^\circ = -116.128 - 2.087\times10^{-3}T - 2.121\times10^{-6}T^2 + 41.400T^{-1}$

$\Delta Gf^\circ = -116.128 + 2.087\times10^{-3}T\ln T + 2.121\times10^{-6}T^2 + 20.700T^{-1} - 9.974\times10^{-3}T$

386.8-458.4 K: $\Delta Hf^\circ = -119.038 - 14.895\times10^{-3}T + 0.863\times10^{-6}T^2 + 41.400T^{-1}$

$\Delta Gf^\circ = -119.038 + 14.895\times10^{-3}T\ln T - 0.863\times10^{-6}T^2 + 20.700T^{-1} - 77.604\times10^{-3}T$

458.4-702.6 K: $\Delta Hf^\circ = -148.465 + 5.785\times10^{-3}T + 0.727\times10^{-6}T^2 + 10.800T^{-1}$

$\Delta Gf^\circ = -148.465 - 5.785\times10^{-3}T\ln T - 0.727\times10^{-6}T^2 + 5.400T^{-1} + 113.321\times10^{-3}T$

702.6-1136 K: $\Delta Hf^\circ = -115.274 + 1.959\times10^{-3}T - 1.078\times10^{-6}T^2 + 15.000T^{-1}$

$\Delta Gf^\circ = -115.274 - 1.959\times10^{-3}T\ln T + 1.078\times10^{-6}T^2 + 7.500T^{-1} + 39.730\times10^{-3}T$

1136-2000 K: $\Delta Hf^\circ = -117.770 + 3.128\times10^{-3}T - 0.947\times10^{-6}T^2 + 69.500T^{-1}$

$\Delta Gf^\circ = -117.770 - 3.128\times10^{-3}T\ln T + 0.947\times10^{-6}T^2 + 34.750T^{-1} + 50.279\times10^{-3}T$

Sources: Enthalpy of formation at 298 K for crystal from Chase (26). Entropy at 298 K and high-temperature data for crystal from Cubicciotti (52). Heat capacity at 298 K estimated. Gas data above sublimation point from Chase (26).

$ZrI_4(g)$

Zirconium Tetraiodide (ideal gas)

[Formation: $Zr(c) + 2I_2(c,l,g) = ZrI_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G°- H°_{298})/T$	$H°- H°_{298}$	ΔHf°	ΔGf°	
298.15	24.997	106.703	106.703	0	-84.900	-97.383	71.382
300	25.007	106.858	106.705	.046	-84.913	-97.460	70.998
386.8	25.309	113.257	107.485	2.233	-85.696	-100.994	57.063
386.8	25.309	113.257	107.485	2.233	-93.114	-100.994	57.063
400	25.355	114.107	107.689	2.567	-93.376	-101.259	55.325
458.4	25.453	117.570	108.731	4.052	-94.528	-102.324	48.784
458.4	25.453	117.570	108.731	4.052	-114.570	-102.324	48.784
500	25.523	119.784	109.560	5.112	-114.534	-101.211	44.239
600	25.616	124.447	111.665	7.669	-114.463	-98.556	35.899
700	25.673	128.400	113.780	10.234	-114.409	-95.909	29.944
800	25.710	131.831	115.827	12.803	-114.377	-93.268	25.479
900	25.736	134.861	117.778	15.375	-114.367	-90.631	22.008
1000	25.754	137.573	119.623	17.950	-114.377	-87.992	19.230
1100	25.768	140.029	121.369	20.526	-114.409	-85.354	16.958
1136	25.772	140.859	121.974	21.454	-114.426	-84.403	16.238
1136	25.772	140.859	121.974	21.454	-115.377	-84.403	16.238
1200	25.778	142.271	123.018	23.103	-115.323	-82.658	15.054
1300	25.786	144.335	124.580	25.682	-115.249	-79.938	13.439
1400	25.793	146.246	126.060	28.261	-115.196	-77.222	12.055
1500	25.798	148.026	127.466	30.840	-115.162	-74.515	10.857
1600	25.802	149.691	128.803	33.420	-115.145	-71.803	9.808
1700	25.806	151.255	130.078	36.001	-115.147	-69.094	8.883
1800	25.809	152.731	131.297	38.581	-115.168	-66.388	8.061
1900	25.811	154.126	132.462	41.162	-115.208	-63.676	7.324
2000	25.813	155.450	133.578	43.744	-115.265	-60.961	6.661

Phase changes: 386.8 K, melting point of I_2; $\Delta H° = 3.709$ kcal/mol.
458.4 K, boiling point of I_2; $\Delta H° = 10.021$ kcal/mol.
1136 K, α - β transition point of Zr; $\Delta H° = 0.951$ kcal/mol.

Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $Cp° = 25.805 + 0.018\times10^{-3}T - 0.723\times10^{5}T^{-2}$

$H°- H°_{298} = 25.805\times10^{-3}T + 0.009\times10^{-6}T^2 + 0.723\times10^{2}T^{-1} - 7.937$

Formation equations (kcal/mol):

298.15-386.8 K: $\Delta Hf° = -82.912 - 5.942\times10^{-3}T - 3.917\times10^{-6}T^2 + 39.400T^{-1}$

$\Delta Gf° = -82.912 + 5.942\times10^{-3}T\ln T + 3.917\times10^{-6}T^2 + 19.700T^{-1} - 83.778\times10^{-3}T$

386.8-458.4 K: $\Delta Hf° = -85.823 - 18.750\times10^{-3}T - 0.933\times10^{-6}T^2 + 39.400T^{-1}$

$\Delta Gf° = -85.823 + 18.750\times10^{-3}T\ln T + 0.933\times10^{-6}T^2 + 19.700T^{-1} - 151.409\times10^{-3}T$

458.4-1136 K: $\Delta Hf° = -115.249 + 1.930\times10^{-3}T - 1.069\times10^{-6}T^2 + 8.800T^{-1}$

$\Delta Gf° = -115.249 - 1.930\times10^{-3}T\ln T + 1.069\times10^{-6}T^2 + 4.400T^{-1} + 39.517\times10^{-3}T$

1136-2000 K: $\Delta Hf° = -117.745 + 3.099\times10^{-3}T - 0.938\times10^{-6}T^2 + 63.300T^{-1}$

$\Delta Gf° = -117.745 - 3.099\times10^{-3}T\ln T + 0.938\times10^{-6}T^2 + 31.650T^{-1} + 50.066\times10^{-3}T$

Sources: Enthalpy of formation at 298 K from Cubicciotti (52). Other data from Chase (26).

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