



Thermodynamic Properties of Sulfides

By L. B. Pankratz, A. D. Mah, and S. W. Watson

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UNIT OF MEASURE ABBREVIATIONS USED IN THIS BULLETIN

atm	atmosphere (1 atm = 101,325 pascals)	K	kelvin, the unit of thermodynamic temperature
cal	thermochemical calorie (1 cal = 4.1840 joules)	kcal/mol	kilocalorie per mole
cal/mol	calorie per mole	mol	mole, gram formula weight or molar mass
cal/mol·K	calorie per mole per kelvin	mol pct	mole percent

OTHER ABBREVIATIONS AND SYMBOLS USED IN THIS BULLETIN

C_p	heat capacity at constant pressure	$\log K$	logarithm (base 10) of the equilibrium constant ($\log K_f =$ equilibrium constant of formation)
S°	entropy standard state	$\ln$	natural logarithm, base $e = 2.7183$
$H - H_{298}$	enthalpy increment between T and 298.15 K	P	pressure in atmospheres
$(G - H_{298})/T$	Gibbs energy function, $[(H - H_{298})/T] - S$	R	gas constant, 1.98719 cal/mol·K
ΔH	enthalpy change ($\Delta H_f =$ enthalpy of formation)	F	Faraday constant, 23,060.9 cal/V-equivalent
ΔG	Gibbs energy change ($\Delta G_f =$ Gibbs energy of formation)		

THERMODYNAMIC PROPERTIES OF SULFIDES

By L. B. Pankratz,¹ A. D. Mah,² and S. W. Watson³

ABSTRACT

Thermodynamic data on the sulfides were reviewed, evaluated, and compiled at the Bureau of Mines Albany Research Center. Values for C_p° , S° , $H^\circ - H_{298}^\circ$, $-(G^\circ - H_{298}^\circ)/T$, ΔH_f° , ΔG_f° , and $\log K_f$ are given in tabular form. C_p° , $H^\circ - H_{298}^\circ$, ΔH_f° , and ΔG_f° are also expressed algebraically.

INTRODUCTION

This compilation is the third 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. The first volume in the present series, Bulletin 672, "Thermodynamic Properties of Elements and Oxides," by L. B. Pankratz (91),⁴ was published in 1982. The second, Bulletin 674, "Thermodynamic Properties of Halides," also by L. B. Pankratz (92), was published in 1984. These works are part of the Bureau's continuing effort to provide information for use as guidelines in mineral technology advancement, pollution control, and energy economy.

The values of standard heat capacities (C_p°), high-temperature relative enthalpies ($H^\circ - H_{298}^\circ$), enthalpies of formation (ΔH_f°), and Gibbs energies of formation (ΔG_f°), are given in both tabular and equation forms. The tables also include standard entropies (S°), Gibbs energy functions [$-(G^\circ - H_{298}^\circ)/T$], and logarithms (base 10) of the

equilibrium constants ($\log K_f$). As a convenience to the user, and since data are available above the boiling point of sulfur for most substances in this compilation, two formation tables are given. The first table, referenced to sulfur in its standard state, $S(c,l)$, terminates at 717.824 K, the normal boiling point of sulfur. The reactions in the second table are referenced to dimeric sulfur vapor, $S_2(g)$, and values are given to the limit of the data. In the latter tables, the symbols ΔH_f° , ΔG_f° , and $\log K_f$ have been replaced with ΔH_r° , ΔG_r° , and $\log K_r$ since these are not standard state formation reactions below 717.824 K.

Where possible, all phases of a sulfide 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 including 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.

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⁴Underlined numbers in parentheses refer to items in the list of references at the end of this bulletin.

METHODS AND CONVENTIONS

The values in this compilation are the result of a review and critical evaluation of relevant thermodynamic data through 1984, though some data published in 1985 have been included. Data for the elements are from Bulletin 672 (91). Most of the data for the actinide sulfides are from Part 4 of the International Atomic Energy Agency series on "The Chemical Thermodynamics of Actinide Elements and Compounds" (47). Mills' compilation, "Thermodynamic Data for Inorganic Sulphides, Selenides, and Tellurides" (80), proved invaluable and is the source of many estimates in this compilation. 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 (59). This program, along with a plot of $(H^\circ - H_{298.15}^\circ)/(T - 298.15)$, which must take the value of C_p° at 298.15 K, was used to merge high-temperature data smoothly with low-temperature heat capacity data. The resulting polynomial was then used in a subroutine of the program to calculate standard heat capacities, entropies, Gibbs energy functions, and relative enthalpies at selected 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.

Tabular values of relative enthalpies are represented by algebraic equations in the form recommended by Maier and Kelley (75). This form was fit to the data by Kelley's method (62). Since the equations 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, $S_8(g)$, 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 derivations.

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 at unit fugacity.

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 or 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 also 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.

THERMODYNAMIC DATA FOR SULFIDES

In the following pages, thermodynamic values for the sulfides 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 298.15 K 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 are also used to denote substances above and below a second order transformation. Again, to avoid confusion, where substances have the same formula but different standard states, the standard state is explicitly given

in the heading; for example, $As_2S_3(c,l)$ and $As_2S_3(vit)$. To avoid repetition, the sources of data for each substance are given only under the table using $S_8(g)$.

Many of the experimental measurements of thermodynamic properties used in this compilation were obtained using the International Practical Temperature Scale for 1948 (IPTS-48). This temperature scale has been superseded by IPTS-68 (22) and the amended edition of 1975 (23). These scales differ by as much as 2.6 K (at 2,000 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.

AgS(g)
Silver Monosulfide (ideal gas)
[Formation: $\text{Ag(c)} + \text{S(c,l)} = \text{AgS(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	8.600	62.440	62.440	0	94.000	80.700	-59.154
300	8.600	62.490	62.440	.016	93.995	80.619	-58.730
368.3	8.702	64.270	62.620	.607	93.785	77.593	-46.043
368.3	8.702	64.270	62.620	.607	93.689	77.593	-46.043
388.36	8.733	64.732	62.718	.782	93.622	76.718	-43.173
388.36	8.733	64.732	62.718	.782	93.209	76.718	-43.173
400	8.750	64.990	62.780	.884	93.151	76.225	-41.647
432.02	8.769	65.665	62.969	1.164	92.970	74.876	-37.878
500	8.810	66.950	63.424	1.763	92.470	72.071	-31.502
600	8.850	68.560	64.150	2.646	91.861	68.051	-24.787
700	8.870	69.930	64.883	3.533	91.297	64.126	-20.021
717.824	8.874	70.153	65.011	3.691	91.200	63.436	-19.314

*Data except enthalpy of formation at 298 K estimated.

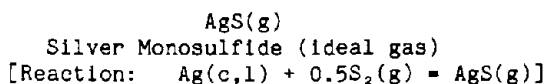
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $C_p^\circ = 8.930 + 0.006 \times 10^{-3}T - 0.295 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 8.930 \times 10^{-3}T + 0.003 \times 10^{-6}T^2 + 0.295 \times 10^{-2}T^{-1} - 2.762$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 95.624 - 4.516 \times 10^{-3}T + 0.802 \times 10^{-6}T^2 - 103.900T^{-1}$
 $\Delta G_f^\circ = 95.624 + 4.516 \times 10^{-3}T \ln T - 0.802 \times 10^{-6}T^2 - 51.950T^{-1} - 74.962 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = 94.509 - 2.253 \times 10^{-3}T - 0.944 \times 10^{-6}T^2 + 51.700T^{-1}$
 $\Delta G_f^\circ = 94.509 + 2.253 \times 10^{-3}T \ln T + 0.944 \times 10^{-6}T^2 + 25.850T^{-1} - 59.779 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = 78.350 + 42.487 \times 10^{-3}T - 44.226 \times 10^{-6}T^2 + 1953.900T^{-1}$
 $\Delta G_f^\circ = 78.350 - 42.487 \times 10^{-3}T \ln T + 44.226 \times 10^{-6}T^2 + 976.950T^{-1} + 225.450 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = 68.872 + 38.581 \times 10^{-3}T - 24.414 \times 10^{-6}T^2 + 5180.400T^{-1}$
 $\Delta G_f^\circ = 68.872 - 38.581 \times 10^{-3}T \ln T + 24.414 \times 10^{-6}T^2 + 2590.200T^{-1} + 223.602 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15*	8.600	62.440	62.440	0	78.645	71.186	-52.180
300	8.600	62.490	62.440	.016	78.643	71.142	-51.826
400	8.750	64.990	62.780	.884	78.500	68.659	-37.513
500	8.810	66.950	63.424	1.763	78.342	66.218	-28.943
600	8.850	68.560	64.150	2.646	78.167	63.810	-23.243
700	8.870	69.930	64.883	3.533	77.972	61.431	-19.179
800	8.890	71.110	65.584	4.421	77.757	59.087	-16.141
900	8.900	72.160	66.260	5.310	77.521	56.762	-13.784
1000	8.910	73.100	66.899	6.201	77.267	54.469	-11.904
1100	8.910	73.950	67.504	7.091	76.989	52.201	-10.371
1200	8.920	74.720	68.068	7.983	76.688	49.968	-9.100
1235.08	8.920	74.977	68.260	8.296	76.575	49.193	-8.705
1235.08	8.920	74.977	68.260	8.296	73.875	49.193	-8.705
1300	8.920	75.440	68.613	8.875	73.640	47.893	-8.052
1400	8.920	76.100	69.124	9.767	73.273	45.929	-7.170
1500	8.930	76.710	69.604	10.659	72.904	43.996	-6.410
1600	8.930	77.290	70.070	11.552	72.531	42.075	-5.747
1700	8.930	77.830	70.509	12.445	72.155	40.185	-5.166
1800	8.930	78.340	70.930	13.338	71.775	38.316	-4.652
1900	8.930	78.830	71.340	14.231	71.393	36.455	-4.193
2000	8.930	79.280	71.717	15.125	71.008	34.643	-3.786

*Data except enthalpy of formation at 298 K estimated.

Phase change: 1235.08 K, melting point of Ag; ΔH° = 2.700 kcal/mol.

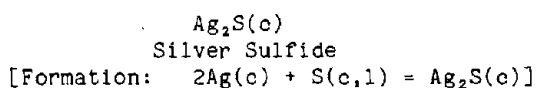
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $\text{Cp}^\circ = 8.930 + 0.006 \times 10^{-3}T - 0.295 \times 10^{-5}T^{-2}$
 $\text{H}^\circ - \text{H}^\circ_{298} = 8.930 \times 10^{-3}T + 0.003 \times 10^{-6}T^2 + 0.295 \times 10^{-2}T^{-1} - 2.762$

Reaction equations (kcal/mol):

298.15-1235.08 K: $\Delta\text{Hr}^\circ = 78.835 - 0.513 \times 10^{-3}T - 1.075 \times 10^{-6}T^2 + 17.550T^{-1}$
 $\Delta\text{Gr}^\circ = 78.835 + 0.513 \times 10^{-3}T \ln T + 1.075 \times 10^{-6}T^2 + 8.775T^{-1} - 28.999 \times 10^{-3}T$
1235.08-2000 K: $\Delta\text{Hr}^\circ = 78.122 - 3.241 \times 10^{-3}T - 0.157 \times 10^{-6}T^2 - 4.650T^{-1}$
 $\Delta\text{Gr}^\circ = 78.122 + 3.241 \times 10^{-3}T \ln T + 0.157 \times 10^{-6}T^2 - 2.325T^{-1} - 46.700 \times 10^{-3}T$

Source: Data from Mills (80) who estimated all except enthalpy of formation at 298 K.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	18.220	34.355	34.355	0	-7.400	-9.294	6.813
300	18.245	34.468	34.355	.034	-7.398	-9.305	6.779
368.3	19.091	38.306	34.740	1.314	-7.336	-9.747	5.784
368.3	19.091	38.306	34.740	1.314	-7.432	-9.747	5.784
388.36	19.340	39.326	34.951	1.699	-7.412	-9.873	5.556
388.36	19.340	39.326	34.951	1.699	-7.825	-9.873	5.556
400	19.484	39.899	35.086	1.925	-7.831	-9.935	5.428
432.02	19.757	41.410	35.500	2.553	-7.862	-10.103	5.111
450	19.910	42.219	35.752	2.910	-7.951	-10.194	4.951
450	19.800	44.337	35.752	3.863	-6.998	-10.194	4.951
500	19.800	46.424	36.718	4.853	-7.086	-10.544	4.609
600	19.800	50.034	38.646	6.833	-7.233	-11.218	4.086
700	19.800	53.086	40.496	8.813	-7.355	-11.873	3.707
717.824	19.800	53.584	40.815	9.166	-7.374	-11.987	3.650

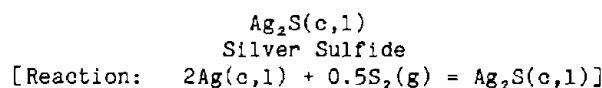
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 450 K, α - β transition point of Ag₂S; ΔH° = 0.953 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-450 K: Cp° = 18.411 + 4.980x10⁻³T - 1.489x10⁻⁵T²
 H° - H°₂₉₈ = 18.411x10⁻³T + 2.490x10⁻⁶T² + 1.489x10⁻²T⁻¹ - 6.210
 450-860 K: Cp° = 19.800
 H° - H°₂₉₈ = 19.800x10⁻³T - 5.047

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -7.646 - 0.307x10⁻³T + 2.371x10⁻⁶T² + 37.700T⁻¹
 ΔGf° = -7.646 + 0.307x10⁻³T ln T - 2.371x10⁻⁶T² + 18.850T⁻¹ - 6.784x10⁻³T
 368.3-388.36 K: ΔHf° = -8.761 + 1.956x10⁻³T + 0.625x10⁻⁶T² + 193.300T⁻¹
 ΔGf° = -8.761 - 1.956x10⁻³T ln T - 0.625x10⁻⁶T² + 96.650T⁻¹ + 8.399x10⁻³T
 388.36-432.02 K: ΔHf° = -24.919 + 46.696x10⁻³T - 42.657x10⁻⁶T² + 2095.500T⁻¹
 ΔGf° = -24.919 - 46.696x10⁻³T ln T + 42.657x10⁻⁶T² + 1047.750T⁻¹ + 293.627x10⁻³T
 432.02-450 K: ΔHf° = -34.398 + 42.790x10⁻³T - 22.845x10⁻⁶T² + 5322.000T⁻¹
 ΔGf° = -34.398 - 42.790x10⁻³T ln T + 22.845x10⁻⁶T² + 2661.000T⁻¹ + 291.780x10⁻³T
 450-717.824 K: ΔHf° = -33.235 + 44.179x10⁻³T - 25.335x10⁻⁶T² + 5173.100T⁻¹
 ΔGf° = -33.235 - 44.179x10⁻³T ln T + 25.335x10⁻⁶T² + 2586.550T⁻¹ + 296.928x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	18.220	34.355	34.355	0	-22.755	-18.808	13.787
300	18.245	34.468	34.355	.034	-22.750	-18.782	13.683
400	19.484	39.899	35.086	1.925	-22.482	-17.501	9.562
450	19.910	42.219	35.752	2.910	-22.322	-16.887	8.201
450	19.800	44.337	35.752	3.863	-21.369	-16.887	8.201
500	19.800	46.424	36.718	4.853	-21.214	-16.398	7.167
600	19.800	50.034	38.646	6.833	-20.927	-15.459	5.631
700	19.800	53.086	40.496	8.813	-20.680	-14.568	4.548
800	19.800	55.730	42.239	10.793	-20.472	-13.710	3.745
860	19.800	57.162	43.231	11.981	-20.366	-13.211	3.357
860	19.800	57.370	43.231	12.160	-20.187	-13.211	3.357
900	19.800	58.270	43.879	12.952	-20.122	-12.887	3.129
1000	19.800	60.356	45.424	14.932	-19.988	-12.089	2.642
1100	19.800	62.243	46.868	16.912	-19.897	-11.302	2.245
1110	19.800	62.422	47.008	17.110	-19.891	-11.224	2.210
1110	22.200	64.098	47.008	18.970	-18.031	-11.224	2.210
1200	22.200	65.829	48.356	20.968	-17.776	-10.684	1.946
1235.08	22.200	66.469	48.861	21.747	-17.689	-10.469	1.853
1235.08	22.200	66.469	48.861	21.747	-23.089	-10.469	1.853
1300	22.200	67.606	49.769	23.188	-22.981	-9.808	1.649
1400	22.200	69.251	51.102	25.408	-22.819	-8.800	1.374

Phase changes: 450 K, α - β transition point of Ag₂S; ΔH° = 0.953 kcal/mol.
860 K, β - γ transition point of Ag₂S; ΔH° = 0.179 kcal/mol.
1110 K, melting point of Ag₂S; ΔH° = 1.860 kcal/mol.
1235.08 K, melting point of Ag; ΔH° = 2.700 kcal/mol.

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

298.15-450 K: Cp° = 18.411 + 4.980x10⁻³T - 1.489x10⁻⁵T²
H° - H°₂₉₈ = 18.411x10⁻³T + 2.490x10⁻⁶T² + 1.489x10⁻²T⁻¹ - 6.210
450-860 K: Cp° = 19.800
H° - H°₂₉₈ = 19.800x10⁻³T - 5.047
860-1110 K: Cp° = 19.800
H° - H°₂₉₈ = 19.800x10⁻³T - 4.868
1110-1400 K: Cp° = 22.200
H° - H°₂₉₈ = 22.200x10⁻³T - 5.672

Reaction equations (kcal/mol):

298.15-450 K: ΔHr° = -24.435 + 3.696x10⁻³T + 0.494x10⁻⁶T² + 159.150T⁻¹
ΔGr° = -24.435 - 3.696x10⁻³TlnT - 0.494x10⁻⁶T² + 79.575T⁻¹ + 39.179x10⁻³T
450-860 K: ΔHr° = -23.271 + 5.085x10⁻³T - 1.996x10⁻⁶T² + 10.250T⁻¹
ΔGr° = -23.271 - 5.085x10⁻³TlnT + 1.996x10⁻⁶T² + 5.125T⁻¹ + 44.327x10⁻³T
860-1110 K: ΔHr° = -23.092 + 5.085x10⁻³T - 1.996x10⁻⁶T² + 10.250T⁻¹
ΔGr° = -23.092 - 5.085x10⁻³TlnT + 1.996x10⁻⁶T² + 5.125T⁻¹ + 44.119x10⁻³T
1110-1235.08 K: ΔHr° = -23.896 + 7.485x10⁻³T - 1.996x10⁻⁶T² + 10.250T⁻¹
ΔGr° = -23.896 - 7.485x10⁻³TlnT + 1.996x10⁻⁶T² + 5.125T⁻¹ + 61.672x10⁻³T
1235.08-1400 K: ΔHr° = -25.323 + 2.029x10⁻³T - 0.160x10⁻⁶T² - 34.150T⁻¹
ΔGr° = -25.323 - 2.029x10⁻³TlnT + 0.160x10⁻⁶T² - 17.075T⁻¹ + 26.268x10⁻³T

Sources: Enthalpy of formation at 298 K based on Kiukkola (69) and Thompson (117). Low-temperature heat capacities and entropy at 298 K based on Walsh (128). High-temperature data based on Thompson (116).

AlS(g)
Aluminum Monosulfide (ideal gas)
[Formation: $\text{Al(c)} + \text{S(c,l)} = \text{AlS(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	7.984	55.092	55.092	0	56.000	43.879	-32.164
300	7.992	55.142	55.092	.015	55.994	43.803	-31.910
368.3	8.228	56.808	55.259	.570	55.760	41.052	-24.360
368.3	8.228	56.808	55.259	.570	55.664	41.052	-24.360
388.36	8.297	57.246	55.351	.736	55.589	40.259	-22.656
388.36	8.297	57.246	55.351	.736	55.176	40.259	-22.656
400	8.337	57.492	55.410	.833	55.114	39.813	-21.752
432.02	8.406	58.137	55.588	1.101	54.922	38.595	-19.524
500	8.553	59.377	56.021	1.678	54.398	36.069	-15.766
600	8.712	60.951	56.716	2.541	53.753	32.466	-11.825
700	8.866	62.306	57.420	3.420	53.150	28.966	-9.043
717.824	8.897	62.529	57.544	3.578	53.046	28.352	-8.632

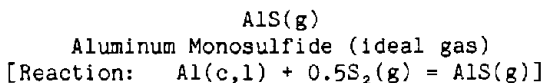
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $\text{Cp}^\circ = 7.598 + 1.956 \times 10^{-3}T - 0.175 \times 10^{-5}T^{-2}$
 $\text{H}^\circ - \text{H}^\circ_{298} = 7.598 \times 10^{-3}T + 0.978 \times 10^{-6}T^2 + 0.175 \times 10^{-2}T^{-1} - 2.411$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta \text{Hf}^\circ = 57.860 - 5.168 \times 10^{-3}T + 0.968 \times 10^{-6}T^2 - 120.700T^{-1}$
 $\Delta \text{Gf}^\circ = 57.860 + 5.168 \times 10^{-3}T \ln T - 0.968 \times 10^{-6}T^2 - 60.350T^{-1} - 75.370 \times 10^{-3}T$
368.3-388.36 K: $\Delta \text{Hf}^\circ = 56.745 - 2.905 \times 10^{-3}T - 0.778 \times 10^{-6}T^2 + 34.900T^{-1}$
 $\Delta \text{Gf}^\circ = 56.745 + 2.905 \times 10^{-3}T \ln T + 0.778 \times 10^{-6}T^2 + 17.450T^{-1} - 60.187 \times 10^{-3}T$
388.36-432.02 K: $\Delta \text{Hf}^\circ = 40.586 + 41.835 \times 10^{-3}T - 44.060 \times 10^{-6}T^2 + 1937.100T^{-1}$
 $\Delta \text{Gf}^\circ = 40.586 - 41.835 \times 10^{-3}T \ln T + 44.060 \times 10^{-6}T^2 + 968.550T^{-1} + 225.041 \times 10^{-3}T$
432.02-717.824 K: $\Delta \text{Hf}^\circ = 31.108 + 37.929 \times 10^{-3}T - 24.248 \times 10^{-6}T^2 + 5163.600T^{-1}$
 $\Delta \text{Gf}^\circ = 31.108 - 37.929 \times 10^{-3}T \ln T + 24.248 \times 10^{-6}T^2 + 2581.800T^{-1} + 223.194 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	7.984	55.092	55.092	0	40.645	34.365	-25.190
300	7.992	55.142	55.092	.015	40.642	34.326	-25.006
400	8.337	57.492	55.410	.833	40.463	32.247	-17.619
500	8.553	59.377	56.021	1.678	40.271	30.216	-13.207
600	8.712	60.951	56.716	2.541	40.059	28.225	-10.281
700	8.866	62.306	57.420	3.420	39.825	26.271	-8.202
800	9.042	63.501	58.107	4.315	39.565	24.351	-6.652
900	9.250	64.577	58.766	5.230	39.281	22.467	-5.456
933.61	9.329	64.918	58.981	5.542	39.179	21.841	-5.113
933.61	9.329	64.918	58.981	5.542	36.599	21.841	-5.113
1000	9.484	65.564	59.398	6.166	36.423	20.796	-4.545
1100	9.733	66.479	60	7.127	36.177	19.246	-3.824
1200	9.984	67.337	60.576	8.113	35.953	17.718	-3.227
1300	10.222	68.146	61.128	9.123	35.750	16.204	-2.724
1400	10.438	68.911	61.657	10.156	35.565	14.710	-2.296
1500	10.625	69.638	62.165	11.210	35.398	13.225	-1.927
1600	10.782	70.329	62.654	12.280	35.244	11.751	-1.605
1700	10.906	70.986	63.124	13.365	35.100	10.288	-1.323
1800	11.000	71.613	63.579	14.461	34.965	8.832	-1.072
1900	11.065	72.209	64.017	15.564	34.834	7.386	-0.850
2000	11.106	72.778	64.441	16.673	34.706	5.944	-0.649

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

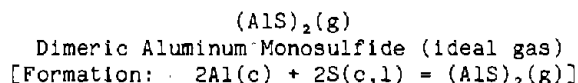
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $\text{Cp}^\circ = 7.598 + 1.956 \times 10^{-3}T - 0.175 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 7.598 \times 10^{-3}T + 0.978 \times 10^{-6}T^2 + 0.175 \times 10^{-2}T^{-1} - 2.411$

Reaction equations (kcal/mol):

298.15-933.61 K: $\Delta\text{Hr}^\circ = 41.071 - 1.166 \times 10^{-3}T - 0.909 \times 10^{-6}T^2 + 0.750T^{-1}$
 $\Delta\text{Gr}^\circ = 41.071 + 1.166 \times 10^{-3}T \ln T + 0.909 \times 10^{-6}T^2 + 0.375T^{-1} - 29.407 \times 10^{-3}T$
 933.61-2000 K: $\Delta\text{Hr}^\circ = 39.803 - 4.164 \times 10^{-3}T + 0.818 \times 10^{-6}T^2 - 16.650T^{-1}$
 $\Delta\text{Gr}^\circ = 39.803 + 4.164 \times 10^{-3}T \ln T - 0.818 \times 10^{-6}T^2 - 8.325T^{-1} - 46.930 \times 10^{-3}T$

Source: Data from Gurvich (50).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	16.495	72.369	72.369	0	24.315	11.347	-8.317
300	16.526	72.471	72.369	.031	24.304	11.267	-8.208
368.3	17.365	75.962	72.719	1.194	23.888	8.341	-4.949
368.3	17.365	75.962	72.719	1.194	23.696	8.341	-4.949
388.36	17.612	76.890	72.911	1.545	23.566	7.510	-4.226
388.36	17.612	76.890	72.911	1.545	22.740	7.510	-4.226
400	17.755	77.412	73.035	1.751	22.628	7.054	-3.854
432.02	17.973	78.788	73.411	2.323	22.279	5.820	-2.944
500	18.435	81.454	74.326	3.564	21.319	3.311	-1.447
600	18.840	84.854	75.806	5.429	20.168	-.178	.065
700	19.098	87.779	77.312	7.327	19.102	-3.483	1.088
717.824	19.129	88.259	77.578	7.668	18.918	-4.055	1.235

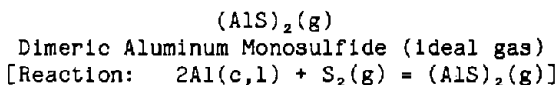
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: $\text{Cp}^\circ = 19.370 + 0.314 \times 10^{-3}T - 2.639 \times 10^{-5}T^{-2}$
 $\text{H}^\circ - \text{H}^\circ_{298} = 19.370 \times 10^{-3}T + 0.157 \times 10^{-6}T^2 + 2.639 \times 10^2 T^{-1} - 6.674$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta \text{Hf}^\circ = 26.182 - 6.162 \times 10^{-3}T + 0.137 \times 10^{-6}T^2 - 12.500T^{-1}$
 $\Delta \text{Gf}^\circ = 26.182 + 6.162 \times 10^{-3}T \ln T - 0.137 \times 10^{-6}T^2 - 6.250T^{-1} - 84.754 \times 10^{-3}T$
 368.3-388.36 K: $\Delta \text{Hf}^\circ = 23.952 - 1.636 \times 10^{-3}T - 3.355 \times 10^{-6}T^2 + 298.700T^{-1}$
 $\Delta \text{Gf}^\circ = 23.952 + 1.636 \times 10^{-3}T \ln T + 3.355 \times 10^{-6}T^2 + 149.350T^{-1} - 54.388 \times 10^{-3}T$
 388.36-432.02 K: $\Delta \text{Hf}^\circ = -8.365 + 87.844 \times 10^{-3}T - 89.919 \times 10^{-6}T^2 + 4103.100T^{-1}$
 $\Delta \text{Gf}^\circ = -8.365 - 87.844 \times 10^{-3}T \ln T + 89.919 \times 10^{-6}T^2 + 2051.550T^{-1} + 516.068 \times 10^{-3}T$
 432.02-717.824 K: $\Delta \text{Hf}^\circ = -27.322 + 80.032 \times 10^{-3}T - 50.295 \times 10^{-6}T^2 + 10556.101T^{-1}$
 $\Delta \text{Gf}^\circ = -27.322 - 80.032 \times 10^{-3}T \ln T + 50.295 \times 10^{-6}T^2 + 5278.050T^{-1} + 512.373 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/T$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHr°	ΔGr°	
298.15	16.495	72.369	72.369	0	-6.395	-7.680	5.630
300	16.526	72.471	72.369	.031	-6.400	-7.688	5.600
400	17.755	77.412	73.035	1.751	-6.674	-8.077	4.413
500	18.435	81.454	74.326	3.564	-6.936	-8.395	3.670
600	18.840	84.854	75.806	5.429	-7.221	-8.660	3.154
700	19.098	87.779	77.312	7.327	-7.548	-8.874	2.770
800	19.272	90.341	78.784	9.246	-7.938	-9.037	2.469
900	19.393	92.618	80.197	11.179	-8.405	-9.150	2.222
933.61	19.423	93.330	80.657	11.831	-8.580	-9.175	2.148
933.61	19.423	93.330	80.657	11.831	-13.740	-9.175	2.148
1000	19.482	94.667	81.543	13.124	-14.047	-8.839	1.932
1100	19.548	96.527	82.822	15.075	-14.509	-8.297	1.649
1200	19.598	98.230	84.036	17.033	-14.971	-7.710	1.404
1300	19.638	99.800	85.189	18.994	-15.437	-7.088	1.192
1400	19.670	101.256	86.285	20.960	-15.906	-6.425	1.003
1500	19.696	102.614	87.329	22.928	-16.380	-5.735	.836
1600	19.717	103.886	88.324	24.899	-16.858	-5.008	.684
1700	19.734	105.082	89.276	26.871	-17.343	-4.255	.547
1800	19.749	106.211	90.185	28.846	-17.830	-3.470	.421
1900	19.761	107.279	91.057	30.821	-18.324	-2.657	.306
2000	19.772	108.293	91.894	32.798	-18.822	-1.820	.199

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

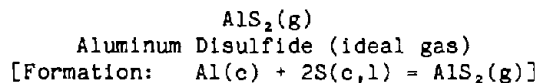
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $\text{Cp}^\circ = 19.370 + 0.314 \times 10^{-3}T - 2.639 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 19.370 \times 10^{-3}T + 0.157 \times 10^{-6}T^2 + 2.639 \times 10^{-2}T^{-1} - 6.674$

Reaction equations (kcal/mol):

298.15-933.61 K: $\Delta\text{Hr}^\circ = -7.396 + 1.843 \times 10^{-3}T - 3.617 \times 10^{-6}T^2 + 230.400T^{-1}$
 $\Delta\text{Gr}^\circ = -7.396 - 1.843 \times 10^{-3}T \ln T + 3.617 \times 10^{-6}T^2 + 115.200T^{-1} + 7.172 \times 10^{-3}T$
 933.61-2000 K: $\Delta\text{Hr}^\circ = -9.931 - 4.153 \times 10^{-3}T - 0.163 \times 10^{-6}T^2 + 195.600T^{-1}$
 $\Delta\text{Gr}^\circ = -9.931 + 4.153 \times 10^{-3}T \ln T + 0.163 \times 10^{-6}T^2 + 97.800T^{-1} - 27.875 \times 10^{-3}T$

Source: Data from Gurvich (50).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	12.131	67.220	67.220	0	58.738	45.285	-33.194
300	12.148	67.295	67.222	.022	58.729	45.201	-32.929
368.3	12.596	69.841	67.478	.870	58.404	42.154	-25.014
368.3	12.596	69.841	67.478	.870	58.212	42.154	-25.014
388.36	12.728	70.513	67.618	1.124	58.106	41.284	-23.232
388.36	12.728	70.513	67.618	1.124	57.280	41.284	-23.232
400	12.804	70.890	67.707	1.273	57.182	40.805	-22.295
432.02	12.919	71.880	67.981	1.685	56.871	39.505	-19.985
500	13.163	73.789	68.641	2.574	55.985	36.848	-16.106
600	13.375	76.210	69.708	3.901	54.947	33.121	-12.064
700	13.510	78.282	70.788	5.246	54.010	29.560	-9.229
717.824	13.526	78.622	70.978	5.487	53.852	28.940	-8.811

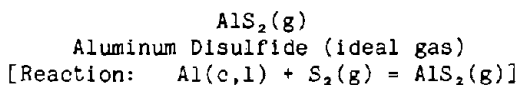
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 13.655 + 0.168x10⁻³T - 1.399x10⁻⁵T⁻²
H° - H₂₉₈° = 13.655x10⁻³T + 0.084x10⁻⁶T² + 1.399x10⁻²T⁻¹ - 4.548

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 61.267 - 7.285x10⁻³T + 1.791x10⁻⁶T² - 153.900T⁻¹
ΔGf° = 61.267 + 7.285x10⁻³TlnT - 1.791x10⁻⁶T² - 76.950T⁻¹ - 93.712x10⁻³T
368.3-388.36 K: ΔHf° = 59.037 - 2.759x10⁻³T - 1.701x10⁻⁶T² + 157.300T⁻¹
ΔGf° = 59.037 + 2.759x10⁻³TlnT + 1.701x10⁻⁶T² + 78.650T⁻¹ - 63.346x10⁻³T
388.36-432.02 K: ΔHf° = 26.720 + 86.721x10⁻³T - 88.265x10⁻⁶T² + 3961.700T⁻¹
ΔGf° = 26.720 - 86.721x10⁻³TlnT + 88.265x10⁻⁶T² + 1980.850T⁻¹ + 507.111x10⁻³T
432.02-717.824 K: ΔHf° = 7.763 + 78.909x10⁻³T - 48.641x10⁻⁶T² + 10414.701T⁻¹
ΔGf° = 7.763 - 78.909x10⁻³TlnT + 48.641x10⁻⁶T² + 5207.351T⁻¹ + 503.416x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	12.131	67.220	67.220	0	28.028	26.258	-19.247
300	12.148	67.295	67.222	.022	28.025	26.247	-19.120
400	12.804	70.890	67.707	1.273	27.880	25.674	-14.027
500	13.163	73.789	68.641	2.574	27.730	25.142	-10.989
600	13.375	76.210	69.708	3.901	27.558	24.640	-8.975
700	13.510	78.282	70.788	5.246	27.360	24.169	-7.546
800	13.600	80.092	71.840	6.602	27.126	23.730	-6.483
900	13.663	81.698	72.848	7.965	26.849	23.319	-5.663
933.61	13.678	82.199	73.176	8.424	26.746	23.189	-5.428
933.61	13.678	82.199	73.176	8.424	24.166	23.189	-5.428
1000	13.709	83.140	73.806	9.334	23.981	23.127	-5.054
1100	13.744	84.448	74.715	10.706	23.699	23.054	-4.580
1200	13.771	85.645	75.577	12.082	23.414	23.010	-4.191
1300	13.793	86.749	76.395	13.460	23.124	22.985	-3.864
1400	13.813	87.771	77.170	14.841	22.829	22.989	-3.589
1500	13.832	88.725	77.910	16.223	22.528	23.008	-3.352
1600	13.850	89.619	78.615	17.607	22.222	23.049	-3.148
1700	13.869	90.459	79.287	18.993	21.910	23.110	-2.971
1800	13.890	91.252	79.929	20.381	21.595	23.192	-2.816
1900	13.912	92.004	80.546	21.771	21.275	23.289	-2.679
2000	13.936	92.718	81.137	23.163	20.951	23.403	-2.557

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

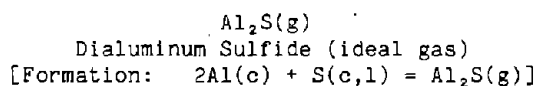
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: Cp° = 13.655 + 0.168x10⁻³T - 1.399x10⁻⁵T⁻²
H° - H°₂₉₈ = 13.655x10⁻³T + 0.084x10⁻⁶T² + 1.399x10⁻³T⁻¹ - 4.548

Reaction equations (kcal/mol):

298.15-933.61 K: ΔHr° = 27.689 + 0.720x10⁻³T - 1.963x10⁻⁶T² + 89.000T⁻¹
ΔGr° = 27.689 - 0.720x10⁻³T ln T + 1.963x10⁻⁶T² + 44.500T⁻¹ - 1.786x10⁻³T
933.61-2000 K: ΔHr° = 26.422 - 2.278x10⁻³T + 0.236x10⁻⁶T² + 71.600T⁻¹
ΔGr° = 26.422 + 2.278x10⁻³T ln T + 0.236x10⁻⁶T² + 35.800T⁻¹ - 19.309x10⁻³T

Source: Data from Gurvich (50).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	13.273	64.824	64.824	0	54.920	41.917	-30.726
300	13.288	64.906	64.824	.025	54.913	41.837	-30.478
368.3	13.688	67.680	65.103	.949	54.642	38.887	-23.075
368.3	13.688	67.680	65.103	.949	54.546	38.887	-23.075
388.36	13.806	68.409	65.255	1.225	54.460	38.037	-21.405
388.36	13.806	68.409	65.255	1.225	54.047	38.037	-21.405
400	13.874	68.818	65.353	1.386	53.978	37.558	-20.521
432.02	13.979	69.890	65.650	1.832	53.766	36.252	-18.339
500	14.203	71.952	66.370	2.791	53.198	33.542	-14.661
600	14.400	74.560	67.523	4.222	52.470	29.683	-10.812
700	14.525	76.790	68.693	5.668	51.752	25.942	-8.099
717.824	14.540	77.155	68.898	5.927	51.623	25.287	-7.699

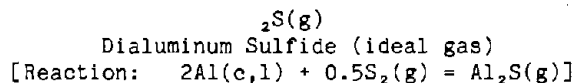
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 14.610 + 0.196x10⁻³T - 1.241x10⁻⁵T⁻²
 H° - H₂₉₈° = 14.610x10⁻³T + 0.098x10⁻⁶T² + 1.241x10⁻²T⁻¹ - 4.781

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 55.874 - 2.748x10⁻³T - 1.639x10⁻⁶T² + 3.300T⁻¹
 ΔGf° = 55.874 + 2.748x10⁻³TlnT + 1.639x10⁻⁶T² + 1.650T⁻¹ - 62.975x10⁻³T
 368.3-388.36 K: ΔHf° = 54.759 - 0.485x10⁻³T - 3.385x10⁻⁶T² + 158.900T⁻¹
 ΔGf° = 54.759 + 0.485x10⁻³TlnT + 3.385x10⁻⁶T² + 79.450T⁻¹ - 47.792x10⁻³T
 388.36-432.02 K: ΔHf° = 38.601 + 44.255x10⁻³T - 46.667x10⁻⁶T² + 2061.100T⁻¹
 ΔGf° = 38.601 - 44.255x10⁻³TlnT + 46.667x10⁻⁶T² + 1030.550T⁻¹ + 237.437x10⁻³T
 432.02-717.824 K: ΔHf° = 29.122 + 40.349x10⁻³T - 26.855x10⁻⁶T² + 5287.600T⁻¹
 ΔGf° = 29.122 - 40.349x10⁻³TlnT + 26.855x10⁻⁶T² + 2643.800T⁻¹ + 235.589x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15	13.273	64.824	64.824	0	39.565	32.404	-23.752
300	13.288	64.906	64.824	.025	39.561	32.360	-23.574
400	13.874	68.818	65.353	1.386	39.327	29.993	-16.387
500	14.203	71.952	66.370	2.791	39.070	27.689	-12.103
600	14.400	74.560	67.523	4.222	38.776	25.442	-9.267
700	14.525	76.790	68.693	5.668	38.427	23.246	-7.258
800	14.610	78.736	69.830	7.125	38.010	21.104	-5.765
900	14.669	80.460	70.916	8.590	37.515	19.020	-4.619
933.61	14.684	80.998	71.269	9.083	37.330	18.332	-4.291
933.61	14.684	80.998	71.269	9.083	32.170	18.332	-4.291
1000	14.713	82.008	71.949	10.059	31.841	17.359	-3.794
1100	14.745	83.412	72.928	11.532	31.348	15.934	-3.166
1200	14.770	84.696	73.856	13.008	30.855	14.557	-2.651
1300	14.789	85.879	74.736	14.486	30.361	13.217	-2.222
1400	14.805	86.976	75.572	15.965	29.864	11.917	-1.860
1500	14.817	87.998	76.367	17.446	29.364	10.650	-1.552
1600	14.828	88.954	77.123	18.929	28.864	9.421	-1.287
1700	14.837	89.853	77.846	20.412	28.360	8.220	-1.057
1800	14.844	90.702	78.538	21.896	27.854	7.050	-0.856
1900	14.850	91.505	79.199	23.381	27.345	5.910	-0.680
2000	14.855	92.266	79.833	24.866	26.833	4.796	-0.524

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

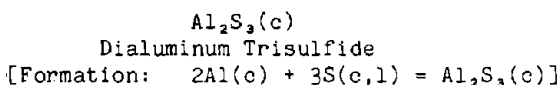
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 14.610 + 0.196 \times 10^{-3}T - 1.241 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 14.610 \times 10^{-3}T + 0.098 \times 10^{-6}T^2 + 1.241 \times 10^{-2}T^{-1} - 4.781$

Reaction equations (kcal/mol):

298.15-933.61 K: $\Delta H_r^\circ = 39.085 + 1.254 \times 10^{-3}T - 3.516 \times 10^{-6}T^2 + 124.750T^{-1}$
 $\Delta G_r^\circ = 39.085 - 1.254 \times 10^{-3}T \ln T + 3.516 \times 10^{-6}T^2 + 62.375T^{-1} - 17.012 \times 10^{-3}T$
 933.61-2000 K: $\Delta H_r^\circ = 36.550 - 4.742 \times 10^{-3}T - 0.062 \times 10^{-6}T^2 + 89.950T^{-1}$
 $\Delta G_r^\circ = 36.550 + 4.742 \times 10^{-3}T \ln T + 0.062 \times 10^{-6}T^2 + 44.975T^{-1} - 52.058 \times 10^{-3}T$

Source: Data from Gurvich (50).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	25.111	27.927	27.927	0	-155.600	-153.034	112.175
300	25.163	28.082	27.927	.047	-155.605	-153.017	111.471
368.3	26.741	33.440	28.464	1.833	-155.782	-152.410	90.439
368.3	26.741	33.440	28.464	1.833	-156.070	-152.410	90.439
388.36	27.204	34.871	28.758	2.374	-156.129	-152.208	85.654
388.36	27.204	34.871	28.758	2.374	-157.368	-152.208	85.654
400	27.473	35.678	28.948	2.692	-157.456	-152.052	83.077
432.02	27.888	37.810	29.527	3.578	-157.753	-151.610	76.695
500	28.768	41.958	30.940	5.509	-158.698	-150.559	65.809
600	29.669	47.287	33.232	8.433	-159.647	-148.836	54.213
700	30.384	51.916	35.577	11.437	-160.407	-146.971	45.886
717.824	30.494	52.681	35.993	11.979	-160.526	-146.626	44.642

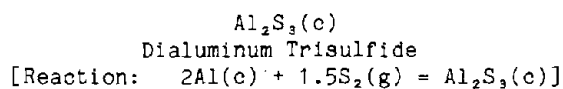
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-900 K: Cp° = 28.152 + 4.312x10⁻³T - 3.846x10⁻⁵T²
 H° - H₂₉₈° = 28.152x10⁻³T + 2.156x10⁻⁶T² + 3.846x10⁻²T⁻¹ - 9.875

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -154.128 - 5.554x10⁻³T + 3.853x10⁻⁶T² - 47.400T⁻¹
 ΔGf° = -154.128 + 5.554x10⁻³TlnT - 3.853x10⁻⁶T² - 23.700T⁻¹ - 26.559x10⁻³T
 368.3-388.36 K: ΔHf° = -157.473 + 1.235x10⁻³T - 1.385x10⁻⁶T² + 419.400T⁻¹
 ΔGf° = -157.473 - 1.235x10⁻³TlnT + 1.385x10⁻⁶T² + 209.700T⁻¹ + 18.989x10⁻³T
 388.36-432.02 K: ΔHf° = -205.948 + 135.455x10⁻³T - 131.231x10⁻⁶T² + 6126.000T⁻¹
 ΔGf° = -205.948 - 135.455x10⁻³TlnT + 131.231x10⁻⁶T² + 3063.000T⁻¹ + 874.674x10⁻³T
 432.02-717.824 K: ΔHf° = -234.384 + 123.737x10⁻³T - 71.795x10⁻⁶T² + 15805.500T⁻¹
 ΔGf° = -234.384 - 123.737x10⁻³TlnT + 71.795x10⁻⁶T² + 7902.750T⁻¹ + 869.132x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15	25.111	27.927	27.927	0	-201.665	-181.574	133.096
300	25.163	28.082	27.927	.047	-201.661	-181.449	132.184
400	27.473	35.678	28.948	2.692	-201.409	-174.749	95.477
500	28.768	41.958	30.940	5.509	-201.081	-168.119	73.484
600	29.669	47.287	33.232	8.433	-200.731	-161.558	58.847
700	30.384	51.916	35.577	11.437	-200.382	-155.057	48.410
800	30.999	56.014	37.880	14.507	-200.057	-148.603	40.596
900	31.558	59.698	40.104	17.635	-199.769	-142.193	34.529

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

298.15-900 K: $C_p^\circ = 28.152 + 4.312 \times 10^{-3}T - 3.846 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 28.152 \times 10^{-3}T + 2.156 \times 10^{-6}T^2 + 3.846 \times 10^{-9}T^3 - 9.875$

Reaction equations (kcal/mol):

298.15-900 K: $\Delta H_r^\circ = -204.494 + 6.453 \times 10^{-3}T - 1.778 \times 10^{-6}T^2 + 316.950T^{-1}$
 $\Delta G_r^\circ = -204.494 - 6.453 \times 10^{-3}T \ln T + 1.778 \times 10^{-6}T^2 + 158.475T^{-1} + 111.329 \times 10^{-3}T$

Source: Data from Ferrante (36).

AsS(g)
 Arsenic Monosulfide (ideal gas)
 [Formation: As(s) + S(c,l) = AsS(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	57.824	57.824	0	45.200	32.788	-24.034
300	8.337	57.875	57.825	.015	45.194	32.711	-23.830
368.3	8.750	59.631	58.000	.601	44.987	29.891	-17.737
368.3	8.750	59.631	58.000	.601	44.891	29.891	-17.737
388.36	8.871	60.098	58.096	.777	44.828	29.076	-16.362
388.36	8.871	60.098	58.096	.777	44.415	29.076	-16.362
400	8.941	60.361	58.159	.881	44.360	28.617	-15.636
432.02	9.068	61.054	58.348	1.169	44.190	27.363	-13.842
500	9.337	62.402	58.808	1.797	43.726	24.756	-10.820
600	9.555	64.126	59.556	2.742	43.187	21.012	-7.654
700	9.653	65.608	60.317	3.704	42.709	17.355	-5.418
717.824	9.657	65.851	60.451	3.876	42.629	16.711	-5.088

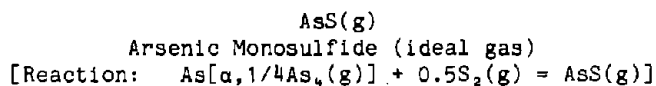
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-3000 K: Cp° = 10.044 - 0.304x10⁻³T - 1.448x10⁻⁵T⁻²
 H° - H₂₉₈° = 10.044x10⁻³T - 0.152x10⁻⁶T² + 1.448x10⁻²T⁻¹ - 3.467

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 46.329 - 3.821x10⁻³T + 0.994x10⁻⁶T² - 23.200T⁻¹
 ΔGf° = 46.329 + 3.821x10⁻³T ln T - 0.994x10⁻⁶T² - 11.600T⁻¹ - 66.758x10⁻³T
 368.3-388.36 K: ΔHf° = 45.214 - 1.558x10⁻³T - 0.752x10⁻⁶T² + 132.400T⁻¹
 ΔGf° = 45.214 + 1.558x10⁻³T ln T + 0.752x10⁻⁶T² + 66.200T⁻¹ - 51.575x10⁻³T
 388.36-432.02 K: ΔHf° = 29.055 + 43.182x10⁻³T - 44.034x10⁻⁶T² + 2034.600T⁻¹
 ΔGf° = 29.055 - 43.182x10⁻³T ln T + 44.034x10⁻⁶T² + 1017.300T⁻¹ + 233.653x10⁻³T
 432.02-717.824 K: ΔHf° = 19.577 + 39.276x10⁻³T - 24.222x10⁻⁶T² + 5261.100T⁻¹
 ΔGf° = 19.577 - 39.276x10⁻³T ln T + 24.222x10⁻⁶T² + 2630.550T⁻¹ + 231.806x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	8.324	57.824	57.824	0	29.845	23.275	-17.061
300	8.337	57.875	57.825	.015	29.842	23.234	-16.926
400	8.941	60.361	58.159	.881	29.709	21.052	-11.502
500	9.337	62.402	58.808	1.797	29.599	18.902	-8.262
600	9.555	64.126	59.556	2.742	29.493	16.771	-6.109
700	9.653	65.608	60.317	3.704	29.384	14.660	-4.577
800	9.678	66.899	61.060	4.671	29.263	12.565	-3.433
876	9.668	67.777	61.605	5.406	29.158	10.981	-2.740
876	9.668	67.777	61.605	5.406	20.849	10.981	-2.740
900	9.665	68.038	61.774	5.638	20.858	10.711	-2.601
1000	9.632	69.055	62.452	6.603	20.886	9.582	-2.094
1100	9.593	69.971	63.095	7.564	20.906	8.450	-1.679
1200	9.552	70.804	63.703	8.521	20.917	7.317	-1.333
1300	9.512	71.567	64.279	9.475	20.922	6.184	-1.040
1400	9.477	72.271	64.825	10.424	20.917	5.050	-.788
1500	9.445	72.924	65.344	11.370	20.906	3.917	-.571
1600	9.416	73.532	65.836	12.313	20.889	2.785	-.380

Phase change: 876 K, sublimation point of As(α) to As₄(g); ΔH° = 33.235 kcal/mol of As₄(g).

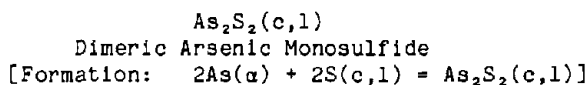
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $\text{Cp}^\circ = 10.044 - 0.304 \times 10^{-3}T - 1.448 \times 10^{-5}T^{-2}$
 $\text{H}^\circ - \text{H}^\circ_{298} = 10.044 \times 10^{-3}T - 0.152 \times 10^{-6}T^2 + 1.448 \times 10^{-2}T^{-1} - 3.467$

Reaction equations (kcal/mol):

298.15-876 K: $\Delta\text{Hr}^\circ = 29.540 + 0.181 \times 10^{-3}T - 0.883 \times 10^{-6}T^2 + 98.250T^{-1}$
 $\Delta\text{Gr}^\circ = 29.540 - 0.181 \times 10^{-3}T \ln T + 0.883 \times 10^{-6}T^2 + 49.125T^{-1} - 20.795 \times 10^{-3}T$
 876-1600 K: $\Delta\text{Hr}^\circ = 20.212 + 0.880 \times 10^{-3}T - 0.305 \times 10^{-6}T^2 + 66.750T^{-1}$
 $\Delta\text{Gr}^\circ = 20.212 - 0.880 \times 10^{-3}T \ln T + 0.305 \times 10^{-6}T^2 + 33.375T^{-1} - 4.891 \times 10^{-3}T$

Source: Data from Mah (73).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	22.480	30.300	30.300	0	-34.000	-33.377	24.466
300*	22.500	30.440	30.300	.042	-34.000	-33.373	24.312
368.3	23.108	35.130	30.781	1.602	-34.025	-33.232	19.720
368.3	23.108	35.130	30.781	1.602	-34.217	-33.232	19.720
388.36	23.286	36.361	31.038	2.067	-34.232	-33.177	18.670
388.36	23.286	36.361	31.038	2.067	-35.058	-33.177	18.670
400	23.390	37.050	31.202	2.339	-35.103	-33.120	18.096
432.02	23.678	38.862	31.704	3.093	-35.265	-32.956	16.672
500	24.290	42.360	32.914	4.723	-35.819	-32.538	14.222
580	25.000	46.020	34.479	6.694	-36.232	-31.983	12.051
580	35.000	48.520	34.479	8.144	-34.782	-31.983	12.051
600	35.000	49.700	34.960	8.844	-34.666	-31.884	11.614
700	35.000	55.100	37.466	12.344	-34.046	-31.473	9.826

*Data above 298 K estimated.

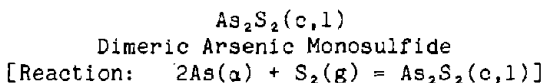
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
580 K, melting point of As₂S₂; ΔH° = 1.450 kcal/mol.

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

298.15-580 K: Cp° = 19.827 + 8.930x10⁻³T
H° - H°₂₉₈ = 19.827x10⁻³T + 4.465x10⁻⁶T² - 6.308
580-700 K: Cp° = 35.000
H° - H°₂₉₈ = 35.000x10⁻³T - 12.156

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -31.117 - 7.903x10⁻³T + 6.757x10⁻⁶T² - 336.000T⁻¹
ΔGf° = -31.117 + 7.903x10⁻³T lnT - 6.757x10⁻⁶T² - 168.000T⁻¹ - 48.702x10⁻³T
368.3-388.36 K: ΔHf° = -33.348 - 3.377x10⁻³T + 3.265x10⁻⁶T² - 24.800T⁻¹
ΔGf° = -33.348 + 3.377x10⁻³T lnT - 3.265x10⁻⁶T² - 12.400T⁻¹ - 18.336x10⁻³T
388.36-432.02 K: ΔHf° = -65.664 + 86.103x10⁻³T - 83.299x10⁻⁶T² + 3779.600T⁻¹
ΔGf° = -65.664 - 86.103x10⁻³T lnT + 83.299x10⁻⁶T² + 1889.800T⁻¹ + 552.121x10⁻³T
432.02-580 K: ΔHf° = -84.622 + 78.291x10⁻³T - 43.675x10⁻⁶T² + 10232.600T⁻¹
ΔGf° = -84.622 - 78.291x10⁻³T lnT + 43.675x10⁻⁶T² + 5116.300T⁻¹ + 548.426x10⁻³T
580-700 K: ΔHf° = -90.470 + 93.464x10⁻³T - 48.140x10⁻⁶T² + 10232.600T⁻¹
ΔGf° = -90.470 - 93.464x10⁻³T lnT + 48.140x10⁻⁶T² + 5116.300T⁻¹ + 652.466x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔH°	ΔG°	
298.15	22.480	30.300	30.300	0	-64.710	-52.404	38.413
300*	22.500	30.440	30.300	.042	-64.704	-52.328	38.120
400	23.390	37.050	31.202	2.339	-64.405	-48.251	26.363
500	24.290	42.360	32.914	4.723	-64.074	-44.245	19.339
580	25.000	46.020	34.479	6.694	-63.781	-41.098	15.486
580	35.000	48.520	34.479	8.144	-62.331	-41.098	15.486
600	35.000	49.700	34.960	8.844	-62.055	-40.366	14.703
700	35.000	55.100	37.466	12.344	-60.696	-36.863	11.509

*Data above 298 K estimated.

Phase change: 580 K, melting point of As_2S_2 ; $\Delta\text{H}^\circ = 1.450$ kcal/mol.

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

298.15-580 K: $\text{Cp}^\circ = 19.827 + 8.930 \times 10^{-3} \text{T}$
 $\text{H}^\circ - \text{H}_{298}^\circ = 19.827 \times 10^{-3} \text{T} + 4.465 \times 10^{-6} \text{T}^2 - 6.308$
 580-700 K: $\text{Cp}^\circ = 35.000$
 $\text{H}^\circ - \text{H}_{298}^\circ = 35.000 \times 10^{-3} \text{T} - 12.156$

Reaction equations (kcal/mol):

298.15-580 K: $\Delta\text{H}^\circ = -64.695 + 0.102 \times 10^{-3} \text{T} + 3.003 \times 10^{-6} \text{T}^2 - 93.100 \text{T}^{-1}$
 $\Delta\text{G}^\circ = -64.695 - 0.102 \times 10^{-3} \text{T} \ln \text{T} - 3.003 \times 10^{-6} \text{T}^2 - 46.550 \text{T}^{-1} + 43.224 \times 10^{-3} \text{T}$
 580-700 K: $\Delta\text{H}^\circ = -70.543 + 15.275 \times 10^{-3} \text{T} - 1.462 \times 10^{-6} \text{T}^2 - 93.100 \text{T}^{-1}$
 $\Delta\text{G}^\circ = -70.543 - 15.275 \times 10^{-3} \text{T} \ln \text{T} + 1.462 \times 10^{-6} \text{T}^2 - 46.550 \text{T}^{-1} + 147.264 \times 10^{-3} \text{T}$

Source: Data from Mills (80) who estimated all above 298 K.

As₂S₃(orpiment, l)
 Diarsenic Trisulfide, Orpiment
 [Formation: 2As(α) + 3S(c, l) = As₂S₃(c, l)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	27.781	39.000	39.000	0	-21.890	-21.577	15.816
300*	27.822	39.172	39.002	.051	-21.891	-21.575	15.717
350	28.566	43.524	39.341	1.464	-21.912	-21.521	13.438
368.3	28.714	44.984	39.586	1.988	-21.923	-21.501	12.759
368.3	28.714	44.984	39.586	1.988	-22.211	-21.501	12.759
388.36	28.877	46.513	39.905	2.566	-22.232	-21.459	12.076
388.36	28.877	46.513	39.905	2.566	-23.471	-21.459	12.076
400	28.971	47.367	40.110	2.903	-23.539	-21.399	11.692
432.02	29.193	49.606	40.732	3.834	-23.787	-21.220	10.735
450	29.317	50.799	41.110	4.360	-24.147	-21.104	10.250
500	29.695	53.907	42.237	5.835	-24.644	-20.738	9.064
550	30.090	56.756	43.429	7.330	-25.081	-20.325	8.076
585	30.336	58.620	44.283	8.387	-25.355	-20.014	7.477
585	45.560	70.370	44.283	15.261	-18.481	-20.014	7.477
600	45.116	71.514	44.949	15.939	-18.365	-20.055	7.305
650	44.569	75.103	47.132	18.181	-17.975	-20.211	6.796
700	44.135	78.390	49.250	20.398	-17.586	-20.399	6.369
717.824	44.010	79.498	49.987	21.183	-17.442	-20.470	6.232

*Data estimated 300-585 K.

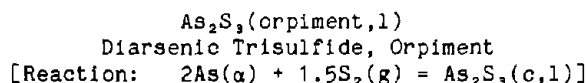
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 585 K, melting point of As₂S₃; ΔH° = 6.874 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-585 K: Cp° = 28.903 + 3.132x10⁻³T - 1.828x10⁻⁶T²
 H° - H₂₉₈° = 28.903x10⁻³T + 1.566x10⁻⁶T² + 1.828x10⁻²T⁻¹ - 9.370
 585-850 K: Cp° = 31.178 + 9.586x10⁻³T + 30.030x10⁻⁵T²
 H° - H₂₉₈° = 31.178x10⁻³T + 4.793x10⁻⁶T² - 30.030x10⁻²T⁻¹ + 0.515

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -19.263 - 7.001x10⁻³T + 5.575x10⁻⁶T² - 308.800T⁻¹
 ΔGf° = -19.263 + 7.001x10⁻³T lnT - 5.575x10⁻⁶T² - 154.400T⁻¹ - 44.251x10⁻³T
 368.3-388.36 K: ΔHf° = -22.608 - 0.212x10⁻³T + 0.337x10⁻⁶T² + 158.000T⁻¹
 ΔGf° = -22.608 + 0.212x10⁻³T lnT - 0.337x10⁻⁶T² + 79.000T⁻¹ + 1.297x10⁻³T
 388.36-432.02 K: ΔHf° = -71.083 + 134.008x10⁻³T - 129.509x10⁻⁶T² + 5864.600T⁻¹
 ΔGf° = -71.083 - 134.008x10⁻³T lnT + 129.509x10⁻⁶T² + 2932.300T⁻¹ + 856.983x10⁻³T
 432.02-585 K: ΔHf° = -99.519 + 122.290x10⁻³T - 70.073x10⁻⁶T² + 15544.100T⁻¹
 ΔGf° = -99.519 - 122.290x10⁻³T lnT + 70.073x10⁻⁶T² + 7772.050T⁻¹ + 851.440x10⁻³T
 585-717.824 K: ΔHf° = -89.634 + 124.565x10⁻³T - 66.846x10⁻⁶T² + 12358.300T⁻¹
 ΔGf° = -89.634 - 124.565x10⁻³T lnT + 66.846x10⁻⁶T² + 6179.150T⁻¹ + 855.581x10⁻³T



T, K	cal/mol·K			kcal/mol			Log. Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	27.781	39.000	39.000	0	-67.955	-50.118	36.737
300*	27.822	39.172	39.002	.051	-67.947	-50.007	36.429
350	28.566	43.524	39.341	1.464	-67.724	-47.036	29.370
400	28.971	47.367	40.110	2.903	-67.492	-44.096	24.093
450	29.317	50.799	41.110	4.360	-67.260	-41.183	20.001
500	29.695	53.907	42.237	5.835	-67.027	-38.298	16.740
550	30.090	56.756	43.429	7.330	-66.789	-35.438	14.081
585	30.336	58.620	44.283	8.387	-66.619	-33.448	12.496
585	45.560	70.370	44.283	15.261	-59.745	-33.448	12.496
600	45.116	71.514	44.949	15.939	-59.448	-32.777	11.939
650	44.569	75.103	47.132	18.181	-58.487	-30.594	10.287
700	44.135	78.390	49.250	20.398	-57.561	-28.484	8.893
750	43.785	81.422	51.294	22.596	-56.664	-26.436	7.703
800	43.498	84.239	53.266	24.778	-55.794	-24.450	6.679
850	43.260	86.868	55.167	26.946	-54.947	-22.522	5.791

*Data estimated 300-585 K.

Phase change: 585 K, melting point of As₂S₃; ΔH° = 6.874 kcal/mol.

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

298.15-585 K: $C_p^\circ = 28.903 + 3.132 \times 10^{-3}T - 1.828 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 28.903 \times 10^{-3}T + 1.566 \times 10^{-6}T^2 + 1.828 \times 10^2 T^{-1} - 9.370$
 585-850 K: $C_p^\circ = 31.178 + 9.586 \times 10^{-3}T + 30.030 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 31.178 \times 10^{-3}T + 4.793 \times 10^{-6}T^2 - 30.030 \times 10^2 T^{-1} + 0.515$

Reaction equations (kcal/mol):

298.15-585 K: $\Delta H_r^\circ = -69.629 + 5.006 \times 10^{-3}T - 0.056 \times 10^{-6}T^2 + 55.550T^{-1}$
 $\Delta G_r^\circ = -69.629 - 5.006 \times 10^{-3}T \ln T + 0.056 \times 10^{-6}T^2 + 27.775T^{-1} + 93.638 \times 10^{-3}T$
 585-850 K: $\Delta H_r^\circ = -59.744 + 7.281 \times 10^{-3}T + 3.171 \times 10^{-6}T^2 - 3130.250T^{-1}$
 $\Delta G_r^\circ = -59.744 - 7.281 \times 10^{-3}T \ln T - 3.171 \times 10^{-6}T^2 - 1565.125T^{-1} + 97.779 \times 10^{-3}T$

Sources: Enthalpy of formation from Johnson (55). Low-temperature heat capacities and entropy at 298 K from Romanovskii (102). Data 300-585 K estimated. Data 585-850 K from Mah (73).

As₂S₃(vitreous,l)
 Diarsenic Trisulfide
 [Formation: 2As(α) + 3S(c,l) = As₂S₃(vit,l)]

T,K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	27.657	40	40	0	-16.630	-16.615	12.179
300	27.689	40.171	40.001	.051	-16.631	-16.615	12.104
368.3	28.562	45.926	40.582	1.968	-16.683	-16.608	9.855
368.3	28.562	45.926	40.582	1.968	-16.971	-16.608	9.855
388.36	28.818	47.448	40.898	2.544	-16.994	-16.585	9.333
388.36	28.818	47.448	40.898	2.544	-18.233	-16.585	9.333
400	28.967	48.301	41.101	2.880	-18.302	-16.536	9.035
432.02	30.065	50.574	41.720	3.825	-18.536	-16.387	8.290
478	31.642	53.657	42.720	5.228	-19.079	-16.117	7.369
500	43.421	55.576	43.242	6.167	-19.052	-15.981	6.985
585	45.560	62.654	45.558	10.001	-18.481	-15.500	5.791
600	45.116	63.799	46.001	10.679	-18.365	-15.426	5.619
700	44.135	70.674	49.048	15.138	-17.586	-14.997	4.682
717.824	44.021	71.782	49.599	15.923	-17.442	-14.932	4.546

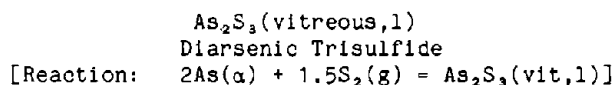
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 478 K, glass transition temperature of As₂S₃.
 585 K, melting point of As₂S₃.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-585 K: Cp° = -62.260 + 177.122x10⁻³T + 32.987x10⁻⁵T⁻²
 H°- H₂₉₈° = -62.260x10⁻³T + 86.561x10⁻⁶T² - 32.987x10⁻²T⁻¹ + 21.754
 585-850 K: Cp° = 31.178 + 9.586x10⁻³T + 30.030x10⁻⁵T⁻²
 H°- H₂₉₈° = 31.178x10⁻³T + 4.793x10⁻⁶T² - 30.030x10⁻²T⁻¹ - 4.745

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 17.121 - 98.164x10⁻³T + 92.570x10⁻⁶T² - 3790.300T⁻¹
 ΔGf° = 17.121 + 98.164x10⁻³TlnT - 92.570x10⁻⁶T² - 1895.150T⁻¹ - 623.532x10⁻³T
 368.3-388.36 K: ΔHf° = 13.776 - 91.375x10⁻³T + 87.332x10⁻⁶T² - 3323.500T⁻¹
 ΔGf° = 13.776 + 91.375x10⁻³TlnT - 87.332x10⁻⁶T² - 1661.750T⁻¹ - 577.983x10⁻³T
 388.36-432.02 K: ΔHf° = -34.699 + 42.845x10⁻³T - 42.514x10⁻⁶T² + 2383.100T⁻¹
 ΔGf° = -34.699 - 42.845x10⁻³TlnT + 42.514x10⁻⁶T² + 1191.550T⁻¹ + 277.702x10⁻³T
 432.02-585 K: ΔHf° = -63.135 + 31.127x10⁻³T + 16.922x10⁻⁶T² + 12062.600T⁻¹
 ΔGf° = -63.135 - 31.127x10⁻³TlnT - 16.922x10⁻⁶T² + 6031.300T⁻¹ + 272.160x10⁻³T
 585-717.824 K: ΔHf° = -89.634 + 124.565x10⁻³T - 66.846x10⁻⁶T² + 12358.300T⁻¹
 ΔGf° = -89.634 - 124.565x10⁻³TlnT + 66.846x10⁻⁶T² + 6179.150T⁻¹ + 863.372x10⁻³T



T,K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(C° - H _{2,98} °)/T	H° - H _{2,98} °	ΔHr°	ΔGr°	
298.15	27.657	40	40	0	-62.695	-45.156	33.100
300	27.689	40.171	40.001	.051	-62.687	-45.047	32.816
400	28.967	48.301	41.101	2.880	-62.255	-39.232	21.435
478	31.642	53.657	42.720	5.228	-61.825	-34.777	15.900
500	43.421	55.576	43.242	6.167	-61.435	-33.540	14.660
585	45.560	62.654	45.558	10.001	-59.745	-28.934	10.809
600	45.116	63.799	46.001	10.679	-59.448	-28.148	10.253
700	44.135	70.674	49.048	15.138	-57.561	-23.083	7.207
800	43.498	76.523	52.126	19.518	-55.794	-18.277	4.993
850	43.260	79.153	53.640	21.686	-54.947	-15.965	4.105

Phase changes: 478 K, glass transition of As₂S₃.
 585 K, melting point of As₂S₃.

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

298.15-585 K: $C_p^\circ = -62.260 + 177.122 \times 10^{-3}T + 32.987 \times 10^{-5}T^2$
 $H^\circ - H_{2,98}^\circ = -62.260 \times 10^{-3}T + 88.561 \times 10^{-6}T^2 - 32.987 \times 10^{-2}T^{-1} + 21.754$
 585-850 K: $C_p^\circ = 31.178 + 9.586 \times 10^{-3}T + 30.030 \times 10^{-5}T^2$
 $H^\circ - H_{2,98}^\circ = 31.178 \times 10^{-3}T + 4.793 \times 10^{-6}T^2 - 30.030 \times 10^{-2}T^{-1} - 4.745$

Reaction equations (kcal/mol):

298.15-585 K: $\Delta H_r^\circ = -33.245 - 86.157 \times 10^{-3}T + 86.939 \times 10^{-6}T^2 - 3425.950T^{-1}$
 $\Delta G_r^\circ = -33.245 + 86.157 \times 10^{-3}T \ln T - 86.939 \times 10^{-6}T^2 - 1712.975T^{-1} - 485.643 \times 10^{-3}T$
 585-850 K: $\Delta H_r^\circ = -59.744 + 7.281 \times 10^{-3}T + 3.171 \times 10^{-6}T^2 - 3130.250T^{-1}$
 $\Delta G_r^\circ = -59.744 - 7.281 \times 10^{-3}T \ln T - 3.171 \times 10^{-6}T^2 - 1565.125T^{-1} + 105.569 \times 10^{-3}T$

Source: Data from Mah (73).

As₄S₄(β,1)
Tetraarsenic Tetrasulfide, Realgar
[Formation: 4As(α) + 4S(c,1) = As₄S₄(β,1)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(C° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	44.960	60.720	60.720	0	-32.200	-30.990	22.716
300	45.025	60.999	60.722	.083	-32.201	-30.983	22.571
368.3	46.499	70.376	61.666	3.208	-32.246	-30.702	18.218
368.3	46.499	70.376	61.666	3.208	-32.630	-30.702	18.218
388.36	46.932	72.854	62.181	4.145	-32.653	-30.594	17.217
388.36	46.932	72.854	62.181	4.145	-34.305	-30.594	17.217
400	47.183	74.244	62.512	4.693	-34.391	-30.482	16.654
432.02	47.777	77.900	63.518	6.213	-34.703	-30.160	15.257
500	49.037	84.977	65.965	9.506	-35.778	-29.345	12.826
580.15	50.397	92.367	69.113	13.491	-36.569	-28.250	10.642
580.15	63.700	103.356	69.113	19.866	-30.194	-28.250	10.642
600	64.206	105.507	70.280	21.136	-30.084	-28.185	10.266
700	68.312	115.684	76.051	27.743	-29.237	-27.929	8.720
717.824	69.346	117.414	77.057	28.970	-29.020	-27.897	8.493

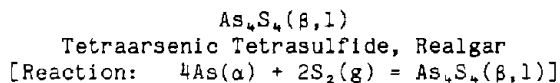
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 580.15 K, melting point of As₄S₄; ΔH° = 6.375 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-580.15 K: Cp° = 41.510 + 15.940x10⁻³T - 1.158x10⁻⁵T⁻²
 H° - H₂₉₈° = 41.510x10⁻³T + 7.970x10⁻⁶T² + 1.158x10⁻²T⁻¹ - 13.473
 580.15-850 K: Cp° = -7.416 + 89.164x10⁻³T + 65.252x10⁻⁵T⁻²
 H° - H₂₉₈° = -7.416x10⁻³T + 44.582x10⁻⁶T² - 65.252x10⁻²T⁻¹ + 20.411

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -27.291 - 13.950x10⁻³T + 12.554x10⁻⁶T² - 556.200T⁻¹
 ΔGf° = -27.291 + 13.950x10⁻³TlnT - 12.554x10⁻⁶T² - 278.100T⁻¹ - 85.014x10⁻³T
 368.3-388.36 K: ΔHf° = -31.752 - 4.898x10⁻³T + 5.570x10⁻⁶T² + 66.200T⁻¹
 ΔGf° = -31.752 + 4.898x10⁻³TlnT - 5.570x10⁻⁶T² + 33.100T⁻¹ - 24.282x10⁻³T
 388.36-432.02 K: ΔHf° = -96.385 + 174.062x10⁻³T - 167.558x10⁻⁶T² + 7675.000T⁻¹
 ΔGf° = -96.385 - 174.062x10⁻³TlnT + 167.558x10⁻⁶T² + 3837.500T⁻¹ + 1116.631x10⁻³T
 432.02-580.15 K: ΔHf° = -134.300 + 158.438x10⁻³T - 88.310x10⁻⁶T² + 20581.000T⁻¹
 ΔGf° = -134.300 - 158.438x10⁻³TlnT + 88.310x10⁻⁶T² + 10290.501T⁻¹ + 1109.241x10⁻³T
 580.15-717.824 K: ΔHf° = -100.416 + 109.512x10⁻³T - 51.698x10⁻⁶T² + 13940.000T⁻¹
 ΔGf° = -100.416 - 109.512x10⁻³TlnT + 51.698x10⁻⁶T² + 6970.000T⁻¹ + 770.612x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	44.960	60.720	60.720	0	-93.620	-69.044	50.610
300	45.025	60.999	60.722	.083	-93.609	-68.892	50.187
400	47.183	74.244	62.512	4.693	-92.995	-60.745	33.189
500	49.037	84.977	65.965	9.506	-92.288	-52.757	23.060
580.15	50.397	92.367	69.113	13.491	-91.666	-46.470	17.506
580.15	63.700	103.356	69.113	19.866	-85.291	-46.470	17.506
600	64.206	105.507	70.280	21.136	-84.862	-45.149	16.445
700	68.312	115.684	76.051	27.743	-82.537	-38.710	12.086
800	74.114	125.171	81.604	34.854	-79.780	-32.629	8.914
850	77.413	129.762	84.302	38.641	-78.196	-29.739	7.646

Phase change: 580.15 K, melting point of As₄S₄; ΔH° = 6.375 kcal/mol.

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

298.15-580.15 K: Cp° = 41.510 + 15.940x10⁻³T - 1.158x10⁻⁵T²
H° - H°₂₉₈ = 41.510x10⁻³T + 7.970x10⁻⁶T² + 1.158x10⁻²T³ - 13.473
580.15-850 K: Cp° = -7.416 + 89.164x10⁻³T + 65.252x10⁻⁵T²
H° - H°₂₉₈ = -7.416x10⁻³T + 44.582x10⁻⁶T² - 65.252x10⁻²T³ + 20.411

Reaction equations (kcal/mol):

298.15-580.15 K: ΔHr° = -94.447 + 2.060x10⁻³T + 5.046x10⁻⁶T² - 70.400T⁻¹
ΔGr° = -94.447 - 2.060x10⁻³T lnT - 5.046x10⁻⁶T² - 35.200T⁻¹ + 98.838x10⁻³T
580.15-850 K: ΔHr° = -60.563 - 46.866x10⁻³T + 41.658x10⁻⁶T² - 6711.400T⁻¹
ΔGr° = -60.563 + 46.866x10⁻³T lnT - 41.658x10⁻⁶T² - 3355.700T⁻¹ - 239.791x10⁻³T

Source: Data from Mah (73).

As₄S₄(g)
Tetraarsenic Tetrasulfide (ideal gas)
[Formation: 4As(α) + 4S(c,l) = As₄S₄(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	39.240	106.590	106.590	0	-.500	-12.966	9.504
300	39.290	106.833	106.590	.073	-.511	-13.043	9.502
368.3	40.534	115.048	107.419	2.810	-.944	-15.853	9.407
368.3	40.534	115.048	107.419	2.810	-1.328	-15.853	9.407
388.36	40.900	117.208	107.870	3.627	-1.471	-16.638	9.363
388.36	40.900	117.208	107.870	3.627	-3.123	-16.638	9.363
400	41.112	118.419	108.159	4.104	-3.280	-17.041	9.311
432.02	41.401	121.596	109.039	5.425	-3.791	-18.125	9.169
500	42.014	127.700	111.170	8.265	-5.319	-20.247	8.850
600	42.521	135.409	114.586	12.494	-7.026	-23.068	8.402
700	42.832	141.989	118.042	16.763	-8.517	-25.623	8.000
717.824	42.869	143.066	118.650	17.527	-8.763	-26.053	7.932

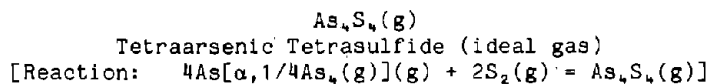
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-3000 K: Cp° = 43.585 + 0.056x10⁻³T - 3.878x10⁵T⁻²
H°- H₂₉₈° = 43.585x10⁻³T + 0.028x10⁻⁶T² + 3.878x10²T⁻¹ - 14.298

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 3.584 - 11.875x10⁻³T + 4.612x10⁻⁶T² - 284.200T⁻¹
ΔGf° = 3.584 + 11.875x10⁻³TlnT - 4.612x10⁻⁶T² - 142.100T⁻¹ - 120.192x10⁻³T
368.3-388.36 K: ΔHf° = -0.877 - 2.823x10⁻³T - 2.372x10⁻⁶T² + 338.200T⁻¹
ΔGf° = -0.877 + 2.823x10⁻³TlnT + 2.372x10⁻⁶T² + 169.100T⁻¹ - 59.461x10⁻³T
388.36-432.02 K: ΔHf° = -65.510 + 176.137x10⁻³T - 175.500x10⁻⁶T² + 7947.000T⁻¹
ΔGf° = -65.510 - 176.137x10⁻³TlnT + 175.500x10⁻⁶T² + 3973.500T⁻¹ + 1081.453x10⁻³T
432.02-717.824 K: ΔHf° = -103.425 + 160.513x10⁻³T - 96.252x10⁻⁶T² + 20853.000T⁻¹
ΔGf° = -103.425 - 160.513x10⁻³TlnT + 96.252x10⁻⁶T² + 10426.500T⁻¹ + 1074.063x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	39.240	106.590	106.590	0	-61.920	-51.020	37.398
300	39.290	106.833	106.590	.073	-61.919	-50.952	37.118
400	41.112	118.419	108.159	4.104	-61.884	-47.304	25.845
500	42.014	127.700	111.170	8.265	-61.829	-43.660	19.084
600	42.521	135.409	114.586	12.494	-61.804	-40.032	14.581
700	42.832	141.989	118.042	16.763	-61.817	-36.403	11.366
800	43.037	147.723	121.402	21.057	-61.877	-32.767	8.952
876	43.144	151.633	123.857	24.332	-61.958	-30.007	7.486
876	43.144	151.633	123.857	24.332	-95.193	-30.007	7.486
900	43.178	152.800	124.613	25.368	-95.054	-28.224	6.854
1000	43.280	157.355	127.663	29.692	-94.476	-20.829	4.552
1100	43.355	161.484	130.554	34.023	-93.911	-13.492	2.681
1200	43.413	165.259	133.291	38.362	-93.352	-6.204	1.130
1300	43.458	168.735	135.884	42.706	-92.806	1.034	-.174
1400	43.493	171.957	138.348	47.053	-92.273	8.234	-1.285
1500	43.522	174.959	140.690	51.404	-91.750	15.396	-2.243
1600	43.546	177.769	142.921	55.757	-91.239	22.519	-3.076

Phase change: 876 K, sublimation point of As(α) to As₄(g); ΔH° = 33.235 kcal/mol of As₄(g).

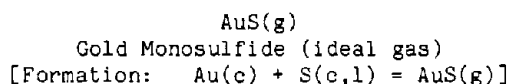
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $C_p^\circ = 43.585 + 0.056 \times 10^{-3}T - 3.878 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 43.585 \times 10^{-3}T + 0.028 \times 10^{-6}T^2 + 3.878 \times 10^{-2}T^{-1} - 14.298$

Reaction equations (kcal/mol):

298.15-876 K: $\Delta H_r^\circ = -63.572 + 4.135 \times 10^{-3}T - 2.896 \times 10^{-6}T^2 + 201.600T^{-1}$
 $\Delta G_r^\circ = -63.572 - 4.135 \times 10^{-3}T \ln T + 2.896 \times 10^{-6}T^2 + 100.800T^{-1} + 63.660 \times 10^{-3}T$
 876-1600 K: $\Delta H_r^\circ = -100.884 + 6.927 \times 10^{-3}T - 0.584 \times 10^{-6}T^2 + 75.600T^{-1}$
 $\Delta G_r^\circ = -100.884 - 6.927 \times 10^{-3}T \ln T + 0.584 \times 10^{-6}T^2 + 37.800T^{-1} + 127.278 \times 10^{-3}T$

Source: Data from Mah (73).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15*	8.490	63.950	63.950	0	55.000	41.595	-30.490
300	8.490	64.000	63.950	.016	54.995	41.514	-30.242
368.3	8.620	65.766	64.132	.602	54.778	38.464	-22.824
368.3	8.620	65.766	64.132	.602	54.682	38.464	-22.824
388.36	8.658	66.224	64.228	.775	54.613	37.583	-21.150
388.36	8.658	66.224	64.228	.775	54.200	37.583	-21.150
400	8.680	66.480	64.290	.876	54.141	37.086	-20.262
432.02	8.709	67.150	64.477	1.154	53.958	35.727	-18.073
500	8.770	68.420	64.922	1.749	53.454	32.905	-14.382
600	8.820	70.030	65.648	2.629	52.843	28.850	-10.508
700	8.850	71.390	66.373	3.512	52.280	24.896	-7.773
717.824	8.854	71.613	66.500	3.670	52.185	24.201	-7.368

*Data except enthalpy of formation at 298 K estimated.

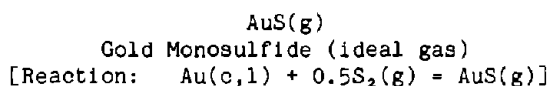
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

$$298.15-2000 \text{ K: } \begin{aligned} C_p^\circ &= 8.920 + 0.012 \times 10^{-3} T - 0.387 \times 10^{-5} T^2 \\ H^\circ - H_{298}^\circ &= 8.920 \times 10^{-3} T + 0.006 \times 10^{-6} T^2 + 0.387 \times 10^{-2} T^{-1} - 2.790 \end{aligned}$$

Formation equations (kcal/mol):

$$\begin{aligned} 298.15-368.3 \text{ K: } \begin{aligned} \Delta H_f^\circ &= 56.634 - 4.663 \times 10^{-3} T + 0.963 \times 10^{-6} T^2 - 98.100 T^{-1} \\ \Delta G_f^\circ &= 56.634 + 4.663 \times 10^{-3} T \ln T - 0.963 \times 10^{-6} T^2 - 49.050 T^{-1} - 76.167 \times 10^{-3} T \end{aligned} \\ 368.3-388.36 \text{ K: } \begin{aligned} \Delta H_f^\circ &= 55.519 - 2.400 \times 10^{-3} T - 0.783 \times 10^{-6} T^2 + 57.500 T^{-1} \\ \Delta G_f^\circ &= 55.519 + 2.400 \times 10^{-3} T \ln T + 0.783 \times 10^{-6} T^2 + 28.750 T^{-1} - 60.984 \times 10^{-3} T \end{aligned} \\ 388.36-432.02 \text{ K: } \begin{aligned} \Delta H_f^\circ &= 39.360 + 42.340 \times 10^{-3} T - 44.065 \times 10^{-6} T^2 + 1959.700 T^{-1} \\ \Delta G_f^\circ &= 39.360 - 42.340 \times 10^{-3} T \ln T + 44.065 \times 10^{-6} T^2 + 979.850 T^{-1} + 224.244 \times 10^{-3} T \end{aligned} \\ 432.02-717.824 \text{ K: } \begin{aligned} \Delta H_f^\circ &= 29.882 + 38.434 \times 10^{-3} T - 24.253 \times 10^{-6} T^2 + 5186.200 T^{-1} \\ \Delta G_f^\circ &= 29.882 - 38.434 \times 10^{-3} T \ln T + 24.253 \times 10^{-6} T^2 + 2593.100 T^{-1} + 222.396 \times 10^{-3} T \end{aligned} \end{aligned}$$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15*	8.490	63.950	63.950	0	39.645	32.082	-23.516
300	8.490	64.000	63.950	.016	39.643	32.037	-23.338
400	8.680	66.480	64.290	.876	39.490	29.520	-16.129
500	8.770	68.420	64.922	1.749	39.327	27.051	-11.824
600	8.820	70.030	65.648	2.629	39.149	24.609	-8.964
700	8.850	71.390	66.373	3.512	38.955	22.201	-6.931
800	8.870	72.570	67.073	4.398	38.750	19.825	-5.416
900	8.880	73.620	67.747	5.286	38.535	17.467	-4.242
1000	8.890	74.550	68.375	6.175	38.311	15.145	-3.310
1100	8.900	75.400	68.978	7.064	38.071	12.838	-2.551
1200	8.910	76.180	69.551	7.955	37.806	10.549	-1.921
1300	8.910	76.890	70.085	8.846	37.486	8.293	-1.394
1337.58	8.914	77.144	70.280	9.181	37.344	7.451	-1.217
1337.58	8.914	77.144	70.280	9.181	34.387	7.451	-1.217
1400	8.920	77.550	70.595	9.737	34.159	6.200	-1.968
1500	8.920	78.170	71.084	10.629	33.792	4.209	-.613
1600	8.920	78.740	71.539	11.522	33.422	2.259	-.309
1700	8.930	79.280	71.978	12.414	33.048	.325	-.042
1800	8.930	79.790	72.397	13.307	32.671	-1.589	.193
1900	8.930	80.280	72.806	14.200	32.291	-3.496	.402
2000	8.930	80.730	73.184	15.093	31.909	-5.354	.585

*Data except enthalpy of formation at 298 K estimated.

Phase change: 1337.58 K, melting point of Au; $\Delta H^\circ = 2.957$ kcal/mol.

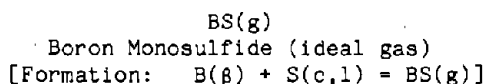
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 8.920 + 0.012 \times 10^{-3}T - 0.387 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 8.920 \times 10^{-3}T + 0.006 \times 10^{-6}T^2 + 0.387 \times 10^{-2}T^{-1} - 2.790$

Reaction equations (kcal/mol):

298.15-1337.58 K: $\Delta H_r^\circ = 39.845 - 0.661 \times 10^{-3}T - 0.914 \times 10^{-6}T^2 + 23.350T^{-1}$
 $\Delta G_r^\circ = 39.845 + 0.661 \times 10^{-3}T \ln T + 0.914 \times 10^{-6}T^2 + 11.675T^{-1} - 30.204 \times 10^{-3}T$
 1337.58-2000 K: $\Delta H_r^\circ = 38.970 - 3.224 \times 10^{-3}T - 0.154 \times 10^{-6}T^2 + 4.550T^{-1}$
 $\Delta G_r^\circ = 38.970 + 3.224 \times 10^{-3}T \ln T + 0.154 \times 10^{-6}T^2 + 2.275T^{-1} - 46.979 \times 10^{-3}T$

Source: Data from Mills (80) who estimated all except enthalpy of formation at 298 K.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	7.182	51.644	51.644	0	58.100	45.407	-33.284
300	7.187	51.688	51.645	.013	58.098	45.329	-33.022
368.3	7.400	53.183	51.796	.511	58.006	42.428	-25.177
368.3	7.400	53.183	51.796	.511	57.910	42.428	-25.177
388.36	7.463	53.577	51.878	.660	57.871	41.587	-23.403
388.36	7.463	53.577	51.878	.660	57.458	41.587	-23.403
400	7.499	53.798	51.931	.747	57.415	41.111	-22.462
432.02	7.595	54.379	52.091	.989	57.272	39.811	-20.139
500	7.799	55.504	52.478	1.513	56.837	37.103	-16.218
600	8.044	56.949	53.107	2.305	56.297	33.205	-12.095
700	8.233	58.203	53.746	3.120	55.794	29.399	-9.179
717.824	8.259	58.410	53.859	3.267	55.708	28.729	-8.747

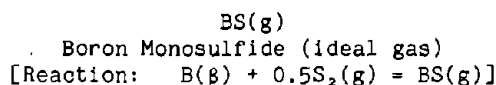
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: $C_p^\circ = 7.805 + 0.734 \times 10^{-3}T - 0.748 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 7.805 \times 10^{-3}T + 0.367 \times 10^{-6}T^2 + 0.748 \times 10^{-2}T^{-1} - 2.611$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 60.508 - 5.092 \times 10^{-3}T + 1.392 \times 10^{-6}T^2 - 302.300T^{-1}$
 $\Delta G_f^\circ = 60.508 + 5.092 \times 10^{-3}T \ln T - 1.392 \times 10^{-6}T^2 - 151.150T^{-1} - 77.547 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = 59.393 - 2.829 \times 10^{-3}T - 0.354 \times 10^{-6}T^2 - 146.700T^{-1}$
 $\Delta G_f^\circ = 59.393 + 2.829 \times 10^{-3}T \ln T + 0.354 \times 10^{-6}T^2 - 73.350T^{-1} - 62.365 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = 43.235 + 41.911 \times 10^{-3}T - 43.636 \times 10^{-6}T^2 + 1755.500T^{-1}$
 $\Delta G_f^\circ = 43.235 - 41.911 \times 10^{-3}T \ln T + 43.636 \times 10^{-6}T^2 + 877.750T^{-1} + 222.864 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = 33.756 + 38.005 \times 10^{-3}T - 23.824 \times 10^{-6}T^2 + 4982.000T^{-1}$
 $\Delta G_f^\circ = 33.756 - 38.005 \times 10^{-3}T \ln T + 23.824 \times 10^{-6}T^2 + 2491.000T^{-1} + 221.016 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	7.182	51.644	51.644	0	42.745	35.893	-26.310
300	7.187	51.688	51.645	.013	42.746	35.852	-26.118
400	7.499	53.798	51.931	.747	42.764	33.546	-18.328
500	7.799	55.504	52.478	1.513	42.709	31.250	-13.659
600	8.044	56.949	53.107	2.305	42.603	28.964	-10.550
700	8.233	58.203	53.746	3.120	42.469	26.704	-8.337
800	8.379	59.313	54.375	3.950	42.318	24.462	-6.683
900	8.491	60.306	54.979	4.794	42.153	22.240	-5.401
1000	8.579	61.206	55.558	5.648	41.975	20.037	-4.379
1100	8.649	62.027	56.110	6.509	41.785	17.846	-3.546
1200	8.706	62.782	56.635	7.377	41.582	15.681	-2.856
1300	8.753	63.481	57.135	8.250	41.367	13.534	-2.275
1400	8.792	64.131	57.611	9.128	41.138	11.402	-1.780
1500	8.825	64.739	58.067	10.008	40.894	9.289	-1.353
1600	8.854	65.309	58.501	10.892	40.634	7.180	-.981
1700	8.880	65.847	58.918	11.779	40.360	5.097	-.655
1800	8.903	66.355	59.317	12.668	40.070	3.044	-.370
1900	8.924	66.837	59.700	13.560	39.767	.997	-.115
2000	8.944	67.295	60.068	14.453	39.448	-1.048	.115

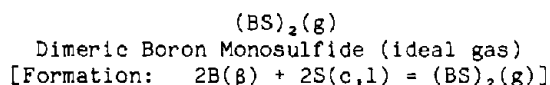
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 7.805 + 0.734 \times 10^{-3}T - 0.748 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 7.805 \times 10^{-3}T + 0.367 \times 10^{-6}T^2 + 0.748 \times 10^{-2}T^{-1} - 2.611$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = 43.720 - 1.090 \times 10^{-3}T - 0.485 \times 10^{-6}T^2 - 180.850T^{-1}$
 $\Delta G_r^\circ = 43.720 + 1.090 \times 10^{-3}T \ln T + 0.485 \times 10^{-6}T^2 - 90.425T^{-1} - 31.584 \times 10^{-3}T$

Source: Data from Chase (19).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	15.653	64.825	64.825	0	33.057	19.138	-14.029
300	15.678	64.922	64.825	.029	33.056	19.054	-13.881
368.3	16.488	68.226	65.157	1.130	32.977	15.868	-9.416
368.3	16.488	68.226	65.157	1.130	32.785	15.868	-9.416
388.36	16.726	69.107	65.339	1.464	32.742	14.950	-8.413
388.36	16.726	69.107	65.339	1.464	31.916	14.950	-8.413
400	16.864	69.603	65.455	1.659	31.852	14.442	-7.891
432.02	17.149	70.913	65.812	2.204	31.628	13.056	-6.605
500	17.754	73.467	66.683	3.392	30.897	10.200	-4.459
600	18.419	76.766	68.096	5.202	30.043	6.138	-2.236
700	18.913	79.644	69.544	7.070	29.275	2.219	-.693
717.824	18.979	80.120	69.801	7.408	29.148	1.532	-.467

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 18.211 + 1.574x10⁻³T - 2.691x10⁻⁵T⁻²
 H° - H₂₉₈° = 18.211x10⁻³T + 0.787x10⁻⁶T² + 2.691x10⁻²T⁻¹ - 6.402

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 36.693 - 7.583x10⁻³T + 2.837x10⁻⁶T² - 485.100T⁻¹
 ΔGf° = 36.693 + 7.583x10⁻³T ln T - 2.837x10⁻⁶T² - 242.550T⁻¹ - 98.508x10⁻³T
 368.3-388.36 K: ΔHf° = 34.462 - 3.057x10⁻³T - 0.655x10⁻⁶T² - 173.900T⁻¹
 ΔGf° = 34.462 + 3.057x10⁻³T ln T + 0.655x10⁻⁶T² - 86.950T⁻¹ - 68.142x10⁻³T
 388.36-432.02 K: ΔHf° = 2.146 + 86.423x10⁻³T - 87.219x10⁻⁶T² + 3630.500T⁻¹
 ΔGf° = 2.146 - 86.423x10⁻³T ln T + 87.219x10⁻⁶T² + 1815.250T⁻¹ + 502.315x10⁻³T
 432.02-717.824 K: ΔHf° = -16.811 + 78.611x10⁻³T - 47.595x10⁻⁶T² + 10083.500T⁻¹
 ΔGf° = -16.811 - 78.611x10⁻³T ln T + 47.595x10⁻⁶T² + 5041.750T⁻¹ + 498.620x10⁻³T

(BS)₂(g)
 Dimeric Boron Monosulfide (ideal gas)
 [Reaction: 2B(s) + S₂(g) = (BS)₂(g)]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	15.653	64.825	64.825	0	2.347	.111	-.081
300	15.678	64.922	64.825	.029	2.352	.100	-.073
400	16.864	69.603	65.455	1.659	2.550	-.689	.377
500	17.754	73.467	66.683	3.392	2.642	-1.506	.658
600	18.419	76.766	68.096	5.202	2.654	-2.344	.854
700	18.913	79.644	69.544	7.070	2.625	-3.172	.990
800	19.283	82.195	70.969	8.981	2.573	-3.993	1.091
900	19.564	84.483	72.345	10.924	2.498	-4.811	1.168
1000	19.779	86.556	73.665	12.891	2.402	-5.617	1.228
1100	19.947	88.449	74.924	14.878	2.286	-6.425	1.276
1200	20.080	90.190	76.123	16.880	2.148	-7.206	1.312
1300	20.187	91.802	77.269	18.893	1.984	-7.974	1.341
1400	20.274	93.301	78.361	20.916	1.794	-8.733	1.363
1500	20.345	94.703	79.405	22.947	1.575	-9.471	1.380
1600	20.405	96.018	80.402	24.985	1.326	-10.223	1.396
1700	20.455	97.256	81.357	27.028	1.046	-10.934	1.406
1800	20.497	98.427	82.274	29.076	.738	-11.606	1.409
1900	20.534	99.536	83.153	31.127	.398	-12.281	1.413
2000	20.565	100.590	83.999	33.182	.028	-12.964	1.417

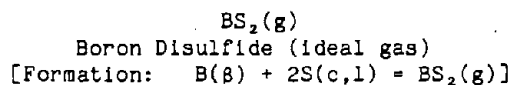
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

$$298.15-2000 \text{ K: } \begin{aligned} C_p^\circ &= 18.211 + 1.574 \times 10^{-3} T - 2.691 \times 10^{-5} T^2 \\ H^\circ - H_{298}^\circ &= 18.211 \times 10^{-3} T + 0.787 \times 10^{-6} T^2 + 2.691 \times 10^2 T^{-1} - 6.402 \end{aligned}$$

Reaction equations (kcal/mol):

$$298.15-2000 \text{ K: } \begin{aligned} \Delta H_r^\circ &= 3.115 + 0.422 \times 10^{-3} T - 0.917 \times 10^{-6} T^2 - 242.200 T^{-1} \\ \Delta G_r^\circ &= 3.115 - 0.422 \times 10^{-3} T \ln T + 0.917 \times 10^{-6} T^2 - 121.100 T^{-1} - 6.582 \times 10^{-3} T \end{aligned}$$

Source: Data from Gurvich (50).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	12.170	61.360	61.360	0	29.000	15.694	-11.504
300	12.190	61.440	61.373	.020	28.995	15.609	-11.371
368.3	12.716	64.000	61.630	.873	28.874	12.570	-7.459
368.3	12.716	64.000	61.630	.873	28.682	12.570	-7.459
388.36	12.870	64.679	61.770	1.130	28.632	11.696	-6.582
388.36	12.870	64.679	61.770	1.130	27.806	11.696	-6.582
400	12.960	65.060	61.860	1.280	27.738	11.213	-6.127
432.02	13.123	66.064	62.135	1.698	27.508	9.898	-5.007
500	13.470	68.010	62.790	2.610	26.787	7.199	-3.147
600	13.820	70.500	63.883	3.970	25.958	3.352	-1.221
700	14.060	72.650	64.979	5.370	25.240	-.351	.109
717.824	14.092	73.004	65.173	5.621	25.121	-1.000	.304

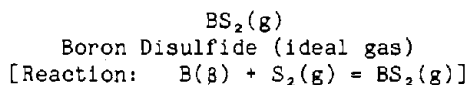
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 14.061 + 0.476x10⁻³T - 1.807x10⁻⁵T⁻²
 H° - H°₂₉₈ = 14.061x10⁻³T + 0.238x10⁻⁶T² + 1.807x10⁻²T⁻¹ - 4.820

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 32.006 - 7.010x10⁻³T + 2.980x10⁻⁶T² - 352.000T⁻¹
 ΔGf° = 32.006 + 7.010x10⁻³T ln T - 2.980x10⁻⁶T² - 176.000T⁻¹ - 91.781x10⁻³T
 368.3-388.36 K: ΔHf° = 29.776 - 2.484x10⁻³T - 0.512x10⁻⁶T² - 40.800T⁻¹
 ΔGf° = 29.776 + 2.484x10⁻³T ln T + 0.512x10⁻⁶T² - 20.400T⁻¹ - 61.415x10⁻³T
 388.36-432.02 K: ΔHf° = -2.541 + 86.996x10⁻³T - 87.076x10⁻⁶T² + 3763.600T⁻¹
 ΔGf° = -2.541 - 86.996x10⁻³T ln T + 87.076x10⁻⁶T² + 1881.800T⁻¹ + 509.042x10⁻³T
 432.02-717.824 K: ΔHf° = -21.498 + 79.184x10⁻³T - 47.452x10⁻⁶T² + 10216.600T⁻¹
 ΔGf° = -21.498 - 79.184x10⁻³T ln T + 47.452x10⁻⁶T² + 5108.300T⁻¹ + 505.347x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	12.170	61.360	61.360	0	-1.710	-3.333	2.443
300	12.190	61.440	61.373	.020	-1.709	-3.345	2.437
400	12.960	65.060	61.860	1.280	-1.564	-3.918	2.141
500	13.470	68.010	62.790	2.610	-1.468	-4.507	1.970
600	13.820	70.500	63.883	3.970	-1.431	-5.129	1.868
700	14.060	72.650	64.979	5.370	-1.410	-5.741	1.792
800	14.240	74.540	66.065	6.780	-1.417	-6.363	1.738
900	14.370	76.220	67.098	8.210	-1.436	-6.978	1.695
1000	14.460	77.740	68.080	9.660	-1.461	-7.584	1.657
1100	14.540	79.120	69.020	11.110	-1.510	-8.198	1.629
1200	14.590	80.390	69.923	12.560	-1.581	-8.811	1.605
1300	14.640	81.560	70.775	14.020	-1.664	-9.409	1.582
1400	14.670	82.650	71.586	15.490	-1.759	-10.002	1.561
1500	14.700	83.660	72.353	16.960	-1.876	-10.578	1.541
1600	14.720	84.610	73.091	18.430	-2.015	-11.167	1.525
1700	14.740	85.500	73.794	19.900	-2.176	-11.732	1.508
1800	14.760	86.340	74.462	21.380	-2.346	-12.266	1.489
1900	14.780	87.140	75.114	22.850	-2.547	-12.820	1.475
2000	14.790	87.900	75.735	24.330	-2.758	-13.370	1.461

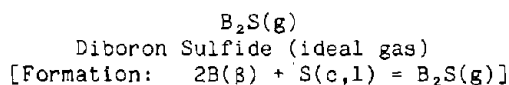
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 14.061 + 0.476 \times 10^{-3}T - 1.807 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 14.061 \times 10^{-3}T + 0.238 \times 10^{-6}T^2 + 1.807 \times 10^{-2}T^{-1} - 4.820$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -1.572 + 0.995 \times 10^{-3}T - 0.774 \times 10^{-6}T^2 - 109.100T^{-1}$
 $\Delta G_r^\circ = -1.572 - 0.995 \times 10^{-3}T \ln T + 0.774 \times 10^{-6}T^2 - 54.550T^{-1} + 0.145 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (126). Other data from Sommer (110).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	12.610	59.304	59.304	0	143.670	129.113	-94.641
300	12.628	59.382	59.305	.023	143.673	129.025	-93.993
368.3	13.137	62.031	59.571	.906	143.760	125.675	-74.575
368.3	13.137	62.031	59.571	.906	143.664	125.675	-74.575
388.36	13.286	62.731	59.717	1.171	143.672	124.696	-70.172
388.36	13.286	62.731	59.717	1.171	143.259	124.696	-70.172
400	13.373	63.125	59.810	1.326	143.242	124.140	-67.826
432.02	13.520	64.160	60.095	1.757	143.167	122.613	-62.026
500	13.831	66.163	60.787	2.688	142.853	119.410	-52.193
600	14.119	68.712	61.900	4.087	142.445	114.755	-41.799
700	14.309	70.904	63.034	5.509	142.031	110.175	-34.398
717.824	14.332	71.264	63.234	5.764	141.958	109.366	-33.297

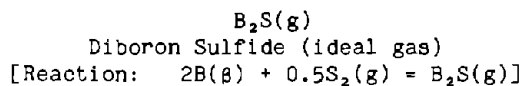
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 14.366 + 0.332x10⁻³T - 1.649x10⁻⁵T⁻²
 H° - H°₂₉₈ = 14.366x10⁻³T + 0.166x10⁻⁶T² + 1.649x10⁻²T⁻¹ - 4.851

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 146.050 - 3.254x10⁻³T + 0.499x10⁻⁶T² - 433.700T⁻¹
 ΔGf° = 146.050 + 3.254x10⁻³T ln T - 0.499x10⁻⁶T² - 216.850T⁻¹ - 72.759x10⁻³T
 368.3-388.36 K: ΔHf° = 144.935 - 0.991x10⁻³T - 1.247x10⁻⁶T² - 278.100T⁻¹
 ΔGf° = 144.935 + 0.991x10⁻³T ln T + 1.247x10⁻⁶T² - 139.050T⁻¹ - 57.576x10⁻³T
 388.36-432.02 K: ΔHf° = 128.777 + 43.749x10⁻³T - 44.529x10⁻⁶T² + 1624.100T⁻¹
 ΔGf° = 128.777 - 43.749x10⁻³T ln T + 44.529x10⁻⁶T² + 812.050T⁻¹ + 227.652x10⁻³T
 432.02-717.824 K: ΔHf° = 119.298 + 39.843x10⁻³T - 24.717x10⁻⁶T² + 4850.600T⁻¹
 ΔGf° = 119.298 - 39.843x10⁻³T ln T + 24.717x10⁻⁶T² + 2425.300T⁻¹ + 225.805x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15	12.610	59.304	59.304	0	128.315	119.600	-87.668
300	12.628	59.382	59.305	.023	128.321	119.548	-87.089
400	13.373	63.125	59.810	1.326	128.591	116.574	-63.692
500	13.831	66.163	60.787	2.688	128.726	113.557	-49.635
600	14.119	68.712	61.900	4.087	128.751	110.514	-40.254
700	14.309	70.904	63.034	5.509	128.706	107.480	-33.556
800	14.439	72.823	64.139	6.947	128.617	104.457	-28.536
900	14.531	74.530	65.201	8.396	128.488	101.443	-24.634
1000	14.598	76.064	66.212	9.852	128.324	98.449	-21.516
1100	14.650	77.458	67.172	11.315	128.132	95.458	-18.966
1200	14.689	78.734	68.082	12.782	127.910	92.502	-16.847
1300	14.720	79.912	68.949	14.252	127.657	89.566	-15.057
1400	14.745	81.003	69.771	15.725	127.376	86.647	-13.526
1500	14.765	82.021	70.554	17.201	127.064	83.756	-12.203
1600	14.781	82.975	71.301	18.678	126.719	80.855	-11.044
1700	14.795	83.871	72.014	20.157	126.344	78.002	-10.028
1800	14.807	84.717	72.696	21.637	125.940	75.194	-9.130
1900	14.816	85.518	73.351	23.118	125.506	72.389	-8.326
2000	14.825	86.278	73.978	24.600	125.042	69.580	-7.603

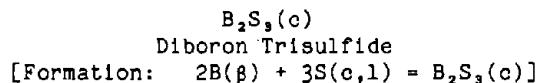
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 14.366 + 0.332 \times 10^{-3}T - 1.649 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 14.366 \times 10^{-3}T + 0.166 \times 10^{-6}T^2 + 1.649 \times 10^{-2}T^{-1} - 4.851$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = 129.262 + 0.749 \times 10^{-3}T - 1.378 \times 10^{-6}T^2 - 312.250T^{-1}$
 $\Delta G_r^\circ = 129.262 - 0.749 \times 10^{-3}T \ln T + 1.378 \times 10^{-6}T^2 - 156.125T^{-1} - 26.796 \times 10^{-3}T$

Source: Data from Gurvich (50).



T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15*	27.990	22.000	22.000	0	-60.300	-59.166	43.369
300	28.020	22.170	22.000	.052	-60.288	-59.156	43.094
368.3	29.065	28.040	22.596	2.005	-59.899	-58.949	34.980
368.3	29.065	28.040	22.596	2.005	-60.187	-58.949	34.980
388.36	29.372	29.590	22.918	2.591	-60.096	-58.882	33.135
388.36	29.372	29.590	22.918	2.591	-61.335	-58.882	33.135
400	29.550	30.460	23.125	2.934	-61.340	-58.809	32.131
432.02	30.040	32.754	23.755	3.888	-61.417	-58.606	29.647
500	31.080	37.220	25.288	5.966	-61.933	-58.108	25.398
600	32.610	43.020	27.770	9.150	-62.270	-57.310	20.875
700	34.140	48.160	30.320	12.488	-62.368	-56.468	17.630
717.824	34.413	49.022	30.774	13.099	-62.359	-56.317	17.146

*Data except enthalpy of formation at 298 K estimated.

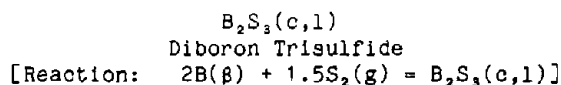
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-836 K: $C_p^\circ = 23.529 + 15.178 \times 10^{-3}T - 0.057 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 23.529 \times 10^{-3}T + 7.589 \times 10^{-6}T^2 + 0.057 \times 10^{-2}T^{-1} - 7.709$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -55.165 - 10.439 \times 10^{-3}T + 11.356 \times 10^{-6}T^2 - 904.100T^{-1}$
 $\Delta G_f^\circ = -55.165 + 10.439 \times 10^{-3}T \ln T - 11.356 \times 10^{-6}T^2 - 452.050T^{-1} - 64.427 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -58.510 - 3.650 \times 10^{-3}T + 6.118 \times 10^{-6}T^2 - 437.300T^{-1}$
 $\Delta G_f^\circ = -58.510 + 3.650 \times 10^{-3}T \ln T - 6.118 \times 10^{-6}T^2 - 218.650T^{-1} - 18.878 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -106.985 + 130.570 \times 10^{-3}T - 123.728 \times 10^{-6}T^2 + 5269.300T^{-1}$
 $\Delta G_f^\circ = -106.985 - 130.570 \times 10^{-3}T \ln T + 123.728 \times 10^{-6}T^2 + 2634.650T^{-1} + 836.807 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -135.421 + 118.852 \times 10^{-3}T - 64.292 \times 10^{-6}T^2 + 14948.800T^{-1}$
 $\Delta G_f^\circ = -135.421 - 118.852 \times 10^{-3}T \ln T + 64.292 \times 10^{-6}T^2 + 7474.400T^{-1} + 831.264 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15*	27.990	22.000	22.000	0	-106.365	-87.707	64.290
300	28.020	22.170	22.000	.052	-106.344	-87.587	63.806
400	29.550	30.460	23.125	2.934	-105.293	-81.506	44.532
500	31.080	37.220	25.288	5.966	-104.315	-75.667	33.074
600	32.610	43.020	27.770	9.150	-103.354	-70.033	25.509
700	34.140	48.160	30.320	12.488	-102.343	-64.554	20.154
800	35.670	52.820	32.847	15.978	-101.252	-59.227	16.180
836	36.220	54.400	33.742	17.272	-100.835	-57.345	14.991
836	36.250	68.160	33.742	28.772	-89.335	-57.345	14.991
900	36.250	70.830	36.283	31.092	-88.595	-54.924	13.337
1000	36.250	74.650	39.933	34.717	-87.477	-51.241	11.199

*Data except enthalpy of formation at 298 K and temperature and enthalpy of fusion estimated.

Phase change: 836 K, melting point of B_2S_3 ; $\Delta H^\circ = 11.500$ kcal/mol.

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

298.15-836 K: $C_p^\circ = 23.529 + 15.178 \times 10^{-3}T - 0.057 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 23.529 \times 10^{-3}T + 7.589 \times 10^{-6}T^2 + 0.057 \times 10^{-3}T^3 - 7.709$
 836-1000 K: $C_p^\circ = 36.250$
 $H^\circ - H_{298}^\circ = 36.250 \times 10^{-3}T - 1.533$

Reaction equations (kcal/mol):

298.15-836 K: $\Delta H_r^\circ = -105.531 + 1.568 \times 10^{-3}T + 5.725 \times 10^{-6}T^2 - 539.750T^{-1}$
 $\Delta G_r^\circ = -105.531 - 1.568 \times 10^{-3}T \ln T - 5.725 \times 10^{-6}T^2 - 269.875T^{-1} + 73.462 \times 10^{-3}T$
 836-1000 K: $\Delta H_r^\circ = -99.355 + 14.289 \times 10^{-3}T - 1.864 \times 10^{-6}T^2 - 545.450T^{-1}$
 $\Delta G_r^\circ = -99.355 - 14.289 \times 10^{-3}T \ln T + 1.864 \times 10^{-6}T^2 - 272.725T^{-1} + 145.329 \times 10^{-3}T$

Source: Data from Mills (80) who estimated all except enthalpy of formation at 298 K and temperature and enthalpy of fusion.

$B_2S_3(g)$
Diboron Trisulfide (ideal gas)
[Formation: $2B(s) + 3S(c,l) = B_2S_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	19.758	83.967	83.967	0	4.240	-13.101	9.603
300	19.785	84.089	83.967	.037	4.238	-13.206	9.620
368.3	20.687	88.243	84.386	1.421	4.057	-17.165	10.186
368.3	20.687	88.243	84.386	1.421	3.769	-17.165	10.186
388.36	20.952	89.347	84.614	1.838	3.692	-18.302	10.299
388.36	20.952	89.347	84.614	1.838	2.453	-18.302	10.299
400	21.106	89.968	84.761	2.083	2.349	-18.923	10.339
432.02	21.437	91.606	85.208	2.764	1.999	-20.614	10.428
500	22.139	94.794	86.298	4.248	.890	-24.072	10.522
600	22.921	98.903	88.065	6.503	-.377	-28.947	10.544
700	23.505	102.483	89.874	8.826	-1.490	-33.616	10.495
717.824	23.583	103.075	90.195	9.246	-1.672	-34.430	10.483

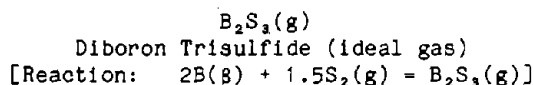
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $C_p^\circ = 22.794 + 1.752 \times 10^{-3}T - 3.164 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 22.794 \times 10^{-3}T + 0.876 \times 10^{-6}T^2 + 3.164 \times 10^{-2}T^3 - 7.935$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 9.150 - 11.174 \times 10^{-3}T + 4.643 \times 10^{-6}T^2 - 593.400T^{-1}$
 $\Delta G_f^\circ = 9.150 + 11.174 \times 10^{-3}T \ln T - 4.643 \times 10^{-6}T^2 - 296.700T^{-1} - 133.572 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = 5.804 - 4.385 \times 10^{-3}T - 0.595 \times 10^{-6}T^2 - 126.600T^{-1}$
 $\Delta G_f^\circ = 5.804 + 4.385 \times 10^{-3}T \ln T + 0.595 \times 10^{-6}T^2 - 63.300T^{-1} - 88.023 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -42.671 + 129.835 \times 10^{-3}T - 130.441 \times 10^{-6}T^2 + 5580.000T^{-1}$
 $\Delta G_f^\circ = -42.671 - 129.835 \times 10^{-3}T \ln T + 130.441 \times 10^{-6}T^2 + 2790.000T^{-1} + 767.662 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -71.107 + 118.117 \times 10^{-3}T - 71.005 \times 10^{-6}T^2 + 15259.500T^{-1}$
 $\Delta G_f^\circ = -71.107 - 118.117 \times 10^{-3}T \ln T + 71.005 \times 10^{-6}T^2 + 7629.750T^{-1} + 762.119 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15	19.758	83.967	83.967	0	-41.824	-41.642	30.524
300	19.785	84.089	83.967	.037	-41.818	-41.637	30.332
400	21.106	89.968	84.761	2.083	-41.604	-41.620	22.740
500	22.139	94.794	86.298	4.248	-41.493	-41.632	18.197
600	22.921	98.903	88.065	6.503	-41.460	-41.669	15.178
700	23.505	102.483	89.874	8.826	-41.464	-41.701	13.020
800	23.944	105.651	91.652	11.199	-41.490	-41.730	11.400
900	24.277	108.491	93.368	13.611	-41.536	-41.759	10.140
1000	24.533	111.063	95.011	16.052	-41.601	-41.779	9.131
1100	24.734	113.411	96.578	18.516	-41.688	-41.805	8.306
1200	24.892	115.570	98.073	20.997	-41.798	-41.807	7.614
1300	25.020	117.568	99.496	23.493	-41.934	-41.797	7.027
1400	25.124	119.426	100.855	26.000	-42.098	-41.780	6.522
1500	25.210	121.162	102.151	28.517	-42.293	-41.743	6.082
1600	25.281	122.792	103.391	31.042	-42.521	-41.724	5.699
1700	25.341	124.326	104.577	33.573	-42.782	-41.664	5.356
1800	25.392	125.776	105.715	36.110	-43.073	-41.565	5.047
1900	25.435	127.150	106.807	38.651	-43.398	-41.471	4.770
2000	25.473	128.456	107.857	41.197	-43.756	-41.386	4.522

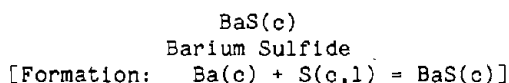
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 22.794 + 1.752 \times 10^{-3}T - 3.164 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 22.794 \times 10^{-3}T + 0.876 \times 10^{-6}T^2 + 3.164 \times 10^2 T^{-1} - 7.935$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -41.217 + 0.834 \times 10^{-3}T - 0.988 \times 10^{-6}T^2 - 229.050T^{-1}$
 $\Delta G_r^\circ = -41.217 - 0.834 \times 10^{-3}T \ln T + 0.988 \times 10^{-6}T^2 - 114.525T^{-1} + 4.317 \times 10^{-3}T$

Source: Data from Gurvich (50).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	11.801	18.737	18.737	0	-110.800	-109.655	80.378
300*	11.809	18.810	18.737	.022	-110.800	-109.647	79.876
368.3	12.090	21.260	18.983	.839	-110.849	-109.383	64.907
368.3	12.090	21.260	18.983	.839	-110.945	-109.383	64.907
388.36	12.172	21.904	19.118	1.082	-110.974	-109.296	61.506
388.36	12.172	21.904	19.118	1.082	-111.387	-109.296	61.506
400	12.220	22.264	19.204	1.224	-111.424	-109.233	59.681
432.02	12.342	23.210	19.466	1.617	-111.560	-109.053	55.167
500	12.600	25.033	20.103	2.465	-112.028	-108.622	47.478
582	12.862	26.967	20.936	3.510	-112.652	-108.016	40.561
600	12.920	27.360	21.123	3.742	-112.723	-107.871	39.292
700	13.160	29.370	22.161	5.046	-113.134	-107.031	33.416
717.824	13.199	29.701	22.345	5.281	-113.212	-106.875	32.539

*Data above 298 K estimated.

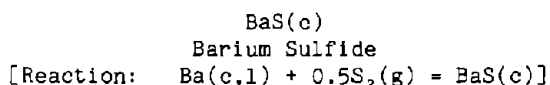
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 11.936 + 1.870x10⁻³T - 0.616x10⁻⁵T²
 H° - H°₂₉₈ = 11.936x10⁻³T + 0.935x10⁻⁶T² + 0.616x10⁻²T⁻¹ - 3.848

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -114.774 + 13.485x10⁻³T - 15.598x10⁻⁶T² + 399.500T⁻¹
 ΔGf° = -114.774 - 13.485x10⁻³TlnT + 15.598x10⁻⁶T² + 199.750T⁻¹ + 87.105x10⁻³T
 368.3-388.36 K: ΔHf° = -115.889 + 15.748x10⁻³T - 17.344x10⁻⁶T² + 555.100T⁻¹
 ΔGf° = -115.889 - 15.748x10⁻³TlnT + 17.344x10⁻⁶T² + 277.550T⁻¹ + 102.288x10⁻³T
 388.36-432.02 K: ΔHf° = -132.047 + 60.488x10⁻³T - 60.626x10⁻⁶T² + 2457.300T⁻¹
 ΔGf° = -132.047 - 60.488x10⁻³TlnT + 60.626x10⁻⁶T² + 1228.650T⁻¹ + 387.516x10⁻³T
 432.02-582 K: ΔHf° = -141.526 + 56.582x10⁻³T - 40.814x10⁻⁶T² + 5683.800T⁻¹
 ΔGf° = -141.526 - 56.582x10⁻³TlnT + 40.814x10⁻⁶T² + 2841.900T⁻¹ + 385.669x10⁻³T
 582-717.824 K: ΔHf° = -138.005 + 44.342x10⁻³T - 27.674x10⁻⁶T² + 5190.300T⁻¹
 ΔGf° = -138.005 - 44.342x10⁻³TlnT + 27.674x10⁻⁶T² + 2595.150T⁻¹ + 310.070x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	11.801	18.737	18.737	0	-126.155	-119.168	87.351
300*	11.809	18.810	18.737	.022	-126.152	-119.124	86.780
400	12.220	22.264	19.204	1.224	-126.075	-116.799	63.815
500	12.600	25.033	20.103	2.465	-126.156	-114.475	50.036
582	12.862	26.967	20.936	3.510	-126.419	-112.542	42.261
600	12.920	27.360	21.123	3.742	-126.418	-112.112	40.836
700	13.160	29.370	22.161	5.046	-126.459	-109.727	34.258
768	13.310	30.597	22.855	5.946	-126.537	-108.097	30.761
800	13.380	31.142	23.176	6.373	-126.574	-107.328	29.320
900	13.570	32.728	24.150	7.720	-126.646	-104.919	25.477
1000	13.780	34.169	25.081	9.088	-126.693	-102.502	22.401
1002	13.784	34.197	25.099	9.116	-126.694	-102.453	22.346
1002	13.784	34.197	25.099	9.116	-128.546	-102.453	22.346
1100	13.965	35.491	25.968	10.475	-128.626	-99.897	19.847
1200	14.150	36.714	26.813	11.881	-128.662	-97.283	17.717
1300	14.336	37.854	27.619	13.305	-128.663	-94.668	15.915
1400	14.520	38.923	28.389	14.748	-128.648	-92.054	14.370
1500	14.699	39.931	29.125	16.209	-128.620	-89.440	13.031
1600	14.880	40.885	29.830	17.688	-128.576	-86.829	11.860
1700	15.066	41.793	30.508	19.185	-128.519	-84.222	10.827
1800	15.250	42.660	31.159	20.701	-128.445	-81.620	9.910
1900	15.429	43.489	31.786	22.235	-128.356	-79.020	9.089
2000	15.610	44.285	32.391	23.787	-128.253	-76.426	8.351

*Data above 298 K estimated.

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: $C_p^\circ = 11.936 + 1.870 \times 10^{-3}T - 0.616 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 11.936 \times 10^{-3}T + 0.935 \times 10^{-6}T^2 + 0.616 \times 10^{-2}T^{-1} - 3.848$

Reaction equations (kcal/mol):

298.15-582 K: $\Delta H_r^\circ = -131.563 + 17.487 \times 10^{-3}T - 17.475 \times 10^{-6}T^2 + 520.950T^{-1}$
 $\Delta G_r^\circ = -131.563 - 17.487 \times 10^{-3}T \ln T + 17.475 \times 10^{-6}T^2 + 260.475T^{-1} + 133.068 \times 10^{-3}T$
582-768 K: $\Delta H_r^\circ = -128.042 + 5.247 \times 10^{-3}T - 4.335 \times 10^{-6}T^2 + 27.450T^{-1}$
 $\Delta G_r^\circ = -128.042 - 5.247 \times 10^{-3}T \ln T + 4.335 \times 10^{-6}T^2 + 13.725T^{-1} + 57.469 \times 10^{-3}T$
768-1002 K: $\Delta H_r^\circ = -125.086 - 2.895 \times 10^{-3}T + 1.256 \times 10^{-6}T^2 + 27.050T^{-1}$
 $\Delta G_r^\circ = -125.086 + 2.895 \times 10^{-3}T \ln T - 1.256 \times 10^{-6}T^2 + 13.525T^{-1} + 3.821 \times 10^{-3}T$
1002-2000 K: $\Delta H_r^\circ = -132.340 + 1.172 \times 10^{-3}T + 0.126 \times 10^{-6}T^2 + 2493.350T^{-1}$
 $\Delta G_r^\circ = -132.340 - 1.172 \times 10^{-3}T \ln T - 0.126 \times 10^{-6}T^2 + 1246.675T^{-1} + 36.802 \times 10^{-3}T$

Source: Data from Chase (17) who estimated those above 298 K.

BaS(g)
Barium Sulfide (ideal gas)
[Formation: Ba(c) + S(c,l) = BaS(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	8.492	59.453	59.453	0	9.030	-1.964	1.440
300	8.497	59.506	59.453	.016	9.024	-2.031	1.480
368.3	8.629	61.265	59.632	.601	8.744	-4.524	2.684
368.3	8.629	61.265	59.632	.601	8.648	-4.524	2.684
388.36	8.668	61.724	59.728	.775	8.549	-5.238	2.948
388.36	8.668	61.724	59.728	.775	8.136	-5.238	2.948
400	8.690	61.980	59.790	.876	8.058	-5.638	3.080
432.02	8.723	62.650	59.977	1.155	7.808	-6.725	3.402
500	8.793	63.931	60.429	1.751	7.088	-8.955	3.914
582	8.844	65.270	61.020	2.474	6.142	-11.515	4.324
600	8.855	65.540	61.152	2.633	5.998	-12.058	4.392
700	8.896	66.908	61.878	3.521	5.171	-15.003	4.684
717.824	8.901	67.132	62.006	3.680	5.017	-15.514	4.723

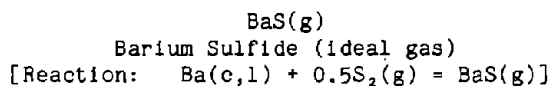
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 582 K, α - β transition point of Ba; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 8.867 + 0.148x10⁻³T - 0.372x10⁻⁵T²
 H° - H₂₉₈° = 8.867x10⁻³T + 0.074x10⁻⁶T² + 0.372x10⁻²T⁻¹ - 2.775

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 6.129 + 10.416x10⁻³T - 16.459x10⁻⁶T² + 375.100T⁻¹
 ΔGf° = 6.129 - 10.416x10⁻³T ln T + 16.459x10⁻⁶T² + 187.550T⁻¹ + 25.183x10⁻³T
 368.3-388.36 K: ΔHf° = 5.014 + 12.679x10⁻³T - 18.205x10⁻⁶T² + 530.700T⁻¹
 ΔGf° = 5.014 - 12.679x10⁻³T ln T + 18.205x10⁻⁶T² + 265.350T⁻¹ + 40.366x10⁻³T
 388.36-432.02 K: ΔHf° = -11.144 + 57.419x10⁻³T - 61.487x10⁻⁶T² + 2432.900T⁻¹
 ΔGf° = -11.144 - 57.419x10⁻³T ln T + 61.487x10⁻⁶T² + 1216.450T⁻¹ + 325.595x10⁻³T
 432.02-582 K: ΔHf° = -20.623 + 53.513x10⁻³T - 41.675x10⁻⁶T² + 5659.400T⁻¹
 ΔGf° = -20.623 - 53.513x10⁻³T ln T + 41.675x10⁻⁶T² + 2829.700T⁻¹ + 323.747x10⁻³T
 582-717.824 K: ΔHf° = -17.102 + 41.273x10⁻³T - 28.535x10⁻⁶T² + 5165.900T⁻¹
 ΔGf° = -17.102 - 41.273x10⁻³T ln T + 28.535x10⁻⁶T² + 2582.950T⁻¹ + 248.148x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	8.492	59.453	59.453	0	-6.325	-11.478	8.413
300	8.497	59.506	59.453	.016	-6.328	-11.509	8.384
400	8.690	61.980	59.790	.876	-6.593	-13.203	7.214
500	8.793	63.931	60.429	1.751	-7.039	-14.808	6.473
582	8.844	65.270	61.020	2.474	-7.625	-16.040	6.023
600	8.855	65.540	61.152	2.633	-7.696	-16.299	5.937
700	8.896	66.908	61.878	3.521	-8.154	-17.698	5.526
768	8.916	67.734	62.361	4.127	-8.526	-18.607	5.295
800	8.925	68.098	62.583	4.412	-8.705	-19.024	5.197
900	8.948	69.151	63.255	5.306	-9.229	-20.283	4.925
1000	8.966	70.095	63.893	6.202	-9.749	-21.483	4.695
1002	8.966	70.113	63.905	6.220	-9.760	-21.507	4.691
1002	8.966	70.113	63.905	6.220	-11.612	-21.507	4.691
1100	8.982	70.950	64.496	7.099	-12.172	-22.448	4.460
1200	8.997	71.732	65.067	7.998	-12.715	-23.358	4.254
1300	9.012	72.453	65.608	8.898	-13.240	-24.224	4.072
1400	9.029	73.121	66.121	9.800	-13.767	-25.049	3.910
1500	9.050	73.745	66.609	10.704	-14.294	-25.836	3.764
1600	9.080	74.330	67.073	11.611	-14.823	-26.588	3.632
1700	9.121	74.881	67.516	12.521	-15.352	-27.306	3.510
1800	9.178	75.404	67.940	13.435	-15.881	-27.995	3.399
1900	9.255	75.903	68.347	14.357	-16.404	-28.654	3.296
2000	9.356	76.380	68.736	15.287	-16.923	-29.286	3.200

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° = 8.867 + 0.148x10⁻³T - 0.372x10⁻⁵T⁻²
H° - H°₂₉₈ = 8.867x10⁻³T + 0.074x10⁻⁶T² + 0.372x10⁻²T⁻¹ - 2.775

Reaction equations (kcal/mol):

298.15-582 K: ΔHr° = -10.659 + 14.418x10⁻³T - 18.336x10⁻⁶T² + 496.550T⁻¹
ΔGr° = -10.659 - 14.418x10⁻³TlnT + 18.336x10⁻⁶T² + 248.275T⁻¹ + 71.146x10⁻³T
582-768 K: ΔHr° = -7.139 + 2.178x10⁻³T - 5.196x10⁻⁶T² + 3.050T⁻¹
ΔGr° = -7.139 - 2.178x10⁻³TlnT + 5.196x10⁻⁶T² + 1.525T⁻¹ - 4.453x10⁻³T
768-1002 K: ΔHr° = -4.183 - 5.964x10⁻³T + 0.395x10⁻⁶T² + 2.650T⁻¹
ΔGr° = -4.183 + 5.964x10⁻³TlnT - 0.395x10⁻⁶T² + 1.325T⁻¹ - 58.101x10⁻³T
1002-2000 K: ΔHr° = -11.437 - 1.897x10⁻³T - 0.735x10⁻⁶T² + 2468.950T⁻¹
ΔGr° = -11.437 + 1.897x10⁻³TlnT + 0.735x10⁻⁶T² + 1234.475T⁻¹ - 25.120x10⁻³T

Source: Data from Chase (17) who estimated some molecular constants.

BeS(c)
Beryllium Sulfide
[Formation: Be(c) + S(c,l) = BeS(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	8.130	8.850	8.850	0	-56.000	-55.678	40.812
300	8.200	8.901	8.851	.015	-56.002	-55.677	40.560
368.3	9.546	10.733	9.029	.628	-56.064	-55.595	32.990
368.3	9.546	10.733	9.029	.628	-56.160	-55.595	32.990
388.36	9.941	11.250	9.131	.823	-56.175	-55.563	31.268
388.36	9.941	11.250	9.131	.823	-56.588	-55.563	31.268
400	10.170	11.547	9.197	.940	-56.613	-55.532	30.341
432.02	10.564	12.345	9.401	1.272	-56.698	-55.443	28.047
500	11.400	13.957	9.913	2.022	-56.969	-55.224	24.138
600	12.200	16.110	10.770	3.204	-57.189	-54.848	19.978
700	12.750	18.033	11.673	4.452	-57.316	-54.451	17.000
717.824	12.827	18.354	11.835	4.680	-57.330	-54.377	16.556

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2500 K: Cp° = 12.598 + 1.500x10⁻³T - 4.369x10⁻⁵T⁻²
H° - H°₂₉₈ = 12.598x10⁻³T + 0.750x10⁻⁶T² + 4.369x10⁻³T⁻¹ - 5.288

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -56.570 - 0.317x10⁻³T + 1.505x10⁻⁶T² + 158.200T⁻¹
ΔGf° = -56.570 + 0.317x10⁻³T ln T - 1.505x10⁻⁶T² + 79.100T⁻¹ + 0.745x10⁻³T
368.3-388.36 K: ΔHf° = -57.685 + 1.946x10⁻³T - 0.241x10⁻⁶T² + 313.800T⁻¹
ΔGf° = -57.685 - 1.946x10⁻³T ln T + 0.241x10⁻⁶T² + 156.900T⁻¹ + 15.928x10⁻³T
388.36-432.02 K: ΔHf° = -73.843 + 46.686x10⁻³T - 43.523x10⁻⁶T² + 2216.000T⁻¹
ΔGf° = -73.843 - 46.686x10⁻³T ln T + 43.523x10⁻⁶T² + 1108.000T⁻¹ + 301.156x10⁻³T
432.02-717.824 K: ΔHf° = -83.322 + 42.780x10⁻³T - 23.711x10⁻⁶T² + 5442.500T⁻¹
ΔGf° = -83.322 - 42.780x10⁻³T ln T + 23.711x10⁻⁶T² + 2721.250T⁻¹ + 299.309x10⁻³T

BeS(c)
Beryllium Sulfide
[Reaction: Be(c,l) + 0.5S₂(g) = BeS(c)]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	8.130	8.850	8.850	0	-71.355	-65.191	47.786
300	8.200	8.901	8.851	.015	-71.354	-65.154	47.464
400	10.170	11.547	9.197	.940	-71.264	-63.098	34.475
500	11.400	13.957	9.913	2.022	-71.097	-61.077	26.697
600	12.200	16.110	10.770	3.204	-70.883	-59.089	21.523
700	12.750	18.033	11.673	4.452	-70.641	-57.146	17.842
800	13.180	19.764	12.576	5.750	-70.377	-55.233	15.089
900	13.540	21.338	13.465	7.086	-70.098	-53.355	12.956
1000	13.840	22.781	14.326	8.455	-69.810	-51.513	11.258
1100	14.094	24.112	15.156	9.852	-69.522	-49.697	9.874
1200	14.320	25.348	15.954	11.273	-69.236	-47.912	8.726
1300	14.522	26.502	16.720	12.716	-68.953	-46.139	7.757
1400	14.690	27.585	17.459	14.177	-68.679	-44.394	6.930
1500	14.807	28.603	18.169	15.651	-68.415	-42.681	6.219
1527	14.838	28.867	18.356	16.051	-68.347	-42.212	6.041
1527	14.838	28.867	18.356	16.051	-68.958	-42.212	6.041
1560	14.875	29.185	18.581	16.542	-68.874	-41.642	5.834
1560	14.875	29.185	18.581	16.542	-71.793	-41.642	5.834
1600	14.920	29.562	18.851	17.138	-71.666	-40.869	5.582
1700	15.024	30.469	19.507	18.635	-71.343	-38.965	5.009
1800	15.130	31.331	20.140	20.143	-71.011	-37.074	4.501
1900	15.241	32.152	20.751	21.661	-70.672	-35.181	4.047
2000	15.350	32.937	21.342	23.191	-70.325	-33.325	3.641
2100	15.455	33.688	21.911	24.731	-69.969	-31.490	3.277
2200	15.560	34.410	22.464	26.282	-69.606	-29.662	2.947
2300	15.665	35.104	22.998	27.843	-69.235	-27.861	2.647
2400	15.770	35.773	23.517	29.415	-68.854	-26.070	2.374
2500	15.875	36.418	24.019	30.997	-68.466	-24.286	2.123

*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:

$$298.15-2500 \text{ K: } \begin{aligned} \text{Cp}^\circ &= 12.598 + 1.500 \times 10^{-3}T - 4.369 \times 10^{-5}T^2 \\ \text{H}^\circ - \text{H}_{298}^\circ &= 12.598 \times 10^{-3}T + 0.750 \times 10^{-6}T^2 + 4.369 \times 10^{-2}T^{-1} - 5.288 \end{aligned}$$

Reaction equations (kcal/mol):

$$\begin{aligned} 298.15-1527 \text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= -73.359 + 3.685 \times 10^{-3}T - 0.372 \times 10^{-6}T^2 + 279.650T^{-1} \\ \Delta \text{Gr}^\circ &= -73.359 - 3.685 \times 10^{-3}T \ln T + 0.372 \times 10^{-6}T^2 + 139.825T^{-1} + 46.708 \times 10^{-3}T \end{aligned} \\ 1527-1560 \text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= -71.775 + 0.726 \times 10^{-3}T + 0.590 \times 10^{-6}T^2 + 402.750T^{-1} \\ \Delta \text{Gr}^\circ &= -71.775 - 0.726 \times 10^{-3}T \ln T - 0.590 \times 10^{-6}T^2 + 201.375T^{-1} + 25.421 \times 10^{-3}T \end{aligned} \\ 1560-2000 \text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= -75.724 + 1.386 \times 10^{-3}T + 0.590 \times 10^{-6}T^2 + 402.750T^{-1} \\ \Delta \text{Gr}^\circ &= -75.724 - 1.386 \times 10^{-3}T \ln T - 0.590 \times 10^{-6}T^2 + 201.375T^{-1} + 32.805 \times 10^{-3}T \end{aligned} \\ 2000-2500 \text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= -74.699 + 0.803 \times 10^{-3}T + 0.700 \times 10^{-6}T^2 - 193.100T^{-1} \\ \Delta \text{Gr}^\circ &= -74.699 - 0.803 \times 10^{-3}T \ln T - 0.700 \times 10^{-6}T^2 - 96.550T^{-1} + 28.152 \times 10^{-3}T \end{aligned} \end{aligned}$$

Source: Data from Chase (17) who estimated all except enthalpy of formation at 298 K.

BeS(g)
Beryllium Sulfide (ideal gas)
[Formation: Be(c) + S(c,l) = BeS(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15*	7.358	50.234	50.234	0	63.000	50.984	-37.372
300	7.365	50.279	50.234	.014	62.997	50.909	-37.087
368.3	7.619	51.816	50.389	.526	62.834	48.172	-28.585
368.3	7.619	51.816	50.389	.526	62.738	48.172	-28.585
388.36	7.694	52.222	50.473	.679	62.682	47.381	-26.663
388.36	7.694	52.222	50.473	.679	62.269	47.381	-26.663
400	7.737	52.450	50.528	.769	62.216	46.936	-25.644
432.02	7.834	53.050	50.692	1.018	62.048	45.718	-23.128
500	8.039	54.211	51.093	1.559	61.568	43.186	-18.876
600	8.264	55.697	51.740	2.374	60.981	39.570	-14.413
700	8.431	56.984	52.400	3.209	60.441	36.040	-11.252
717.824	8.455	57.196	52.516	3.359	60.349	35.421	-10.784

*Data estimated.

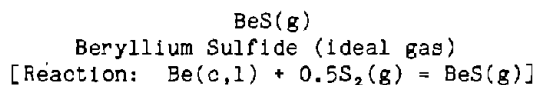
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2500 K: $C_p^\circ = 6.222 + 2.932 \times 10^{-3}T + 0.233 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 6.222 \times 10^{-3}T + 1.466 \times 10^{-6}T^2 - 0.233 \times 10^2 T^{-1} - 1.907$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 65.811 - 6.693 \times 10^{-3}T + 2.221 \times 10^{-6}T^2 - 302.000T^{-1}$
 $\Delta G_f^\circ = 65.811 + 6.693 \times 10^{-3}T \ln T - 2.221 \times 10^{-6}T^2 - 151.000T^{-1} - 85.504 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = 64.696 - 4.430 \times 10^{-3}T + 0.475 \times 10^{-6}T^2 - 146.400T^{-1}$
 $\Delta G_f^\circ = 64.696 + 4.430 \times 10^{-3}T \ln T - 0.475 \times 10^{-6}T^2 - 73.200T^{-1} - 70.321 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = 48.538 + 40.310 \times 10^{-3}T - 42.807 \times 10^{-6}T^2 + 1755.800T^{-1}$
 $\Delta G_f^\circ = 48.538 - 40.310 \times 10^{-3}T \ln T + 42.807 \times 10^{-6}T^2 + 877.900T^{-1} + 214.907 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = 39.059 + 36.404 \times 10^{-3}T - 22.995 \times 10^{-6}T^2 + 4982.300T^{-1}$
 $\Delta G_f^\circ = 39.059 - 36.404 \times 10^{-3}T \ln T + 22.995 \times 10^{-6}T^2 + 2491.150T^{-1} + 213.060 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	7.358	50.234	50.234	0	47.645	41.470	-30.398
300	7.365	50.279	50.234	.014	47.645	41.432	-30.182
400	7.737	52.450	50.528	.769	47.565	39.370	-21.510
500	8.039	54.211	51.093	1.559	47.440	37.333	-16.318
600	8.264	55.697	51.740	2.374	47.287	35.329	-12.868
700	8.431	56.984	52.400	3.209	47.116	33.345	-10.411
800	8.565	58.119	53.045	4.059	46.932	31.392	-8.576
900	8.691	59.135	53.666	4.922	46.738	29.464	-7.155
1000	8.834	60.058	54.260	5.798	46.533	27.553	-6.022
1100	9.014	60.908	54.826	6.690	46.316	25.665	-5.099
1200	9.247	61.702	55.366	7.603	46.094	23.793	-4.333
1300	9.541	62.453	55.883	8.541	45.872	21.949	-3.690
1400	9.896	63.173	56.378	9.513	45.658	20.119	-3.141
1500	10.307	63.869	56.854	10.522	45.456	18.291	-2.665
1527	10.429	64.054	56.980	10.802	45.404	17.809	-2.549
1527	10.429	64.054	56.980	10.802	44.793	17.809	-2.549
1560	10.578	64.279	57.132	11.149	44.733	17.218	-2.412
1560	10.578	64.279	57.132	11.149	41.814	17.218	-2.412
1600	10.759	64.549	57.314	11.576	41.772	16.590	-2.266
1700	11.237	65.215	57.759	12.675	41.698	15.007	-1.929
1800	11.722	65.871	58.192	13.823	41.669	13.434	-1.631
1900	12.195	66.518	58.613	15.019	41.686	11.882	-1.367
2000	12.639	67.155	59.024	16.261	41.746	10.310	-1.127
2100	13.042	67.781	59.426	17.546	41.845	8.730	-.908
2200	13.391	68.396	59.820	18.868	41.980	7.155	-.711
2300	13.683	68.998	60.206	20.222	42.144	5.562	-.528
2400	13.912	69.586	60.585	21.602	42.332	3.966	-.361
2500	14.082	70.157	60.956	23.002	42.539	2.372	-.207

*Data 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:

298.15-2500 K: $C_p^\circ = 6.222 + 2.932 \times 10^{-3}T + 0.233 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 6.222 \times 10^{-3}T + 1.466 \times 10^{-6}T^2 - 0.233 \times 10^{-2}T^{-1} - 1.907$

Reaction equations (kcal/mol):

298.15-1527 K: $\Delta H_r^\circ = 49.022 - 2.690 \times 10^{-3}T + 0.344 \times 10^{-6}T^2 - 180.550T^{-1}$
 $\Delta G_r^\circ = 49.022 + 2.690 \times 10^{-3}T \ln T - 0.344 \times 10^{-6}T^2 - 90.275T^{-1} - 39.541 \times 10^{-3}T$
1527-1560 K: $\Delta H_r^\circ = 50.606 - 5.649 \times 10^{-3}T + 1.306 \times 10^{-6}T^2 - 57.450T^{-1}$
 $\Delta G_r^\circ = 50.606 + 5.649 \times 10^{-3}T \ln T - 1.306 \times 10^{-6}T^2 - 28.725T^{-1} - 60.828 \times 10^{-3}T$
1560-2000 K: $\Delta H_r^\circ = 46.657 - 4.990 \times 10^{-3}T + 1.306 \times 10^{-6}T^2 - 57.450T^{-1}$
 $\Delta G_r^\circ = 46.657 + 4.990 \times 10^{-3}T \ln T - 1.306 \times 10^{-6}T^2 - 28.725T^{-1} - 53.445 \times 10^{-3}T$
2000-2500 K: $\Delta H_r^\circ = 47.682 - 5.573 \times 10^{-3}T + 1.416 \times 10^{-6}T^2 - 653.300T^{-1}$
 $\Delta G_r^\circ = 47.682 + 5.573 \times 10^{-3}T \ln T - 1.416 \times 10^{-6}T^2 - 326.650T^{-1} - 58.098 \times 10^{-3}T$

Source: Data are those estimated by Chase (17):

BiS(g)
Bismuth Monosulfide (ideal gas)
[Formation: $\text{Bi(c,l)} + \text{S(c,l)} = \text{BiS(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	8.436	61.599	61.599	0	40.800	28.761	-21.082
300	8.441	61.652	61.599	.016	40.795	28.688	-20.899
368.3	8.589	63.401	61.776	.599	40.573	25.953	-15.400
368.3	8.589	63.401	61.776	.599	40.477	25.953	-15.400
388.36	8.633	63.858	61.871	.771	40.404	25.164	-14.161
388.36	8.633	63.858	61.871	.771	39.991	25.164	-14.161
400	8.658	64.113	61.933	.872	39.930	24.720	-13.506
432.02	8.696	64.781	62.120	1.150	39.739	23.510	-11.893
500	8.776	66.059	62.571	1.744	39.207	21.001	-9.179
544.59	8.808	66.810	62.888	2.136	38.892	19.389	-7.781
544.59	8.808	66.810	62.888	2.136	36.192	19.389	-7.781
600	8.847	67.666	63.291	2.625	35.823	17.695	-6.445
700	8.895	69.033	64.014	3.513	35.218	14.724	-4.597
717.824	8.901	69.257	64.142	3.672	35.118	14.204	-4.325

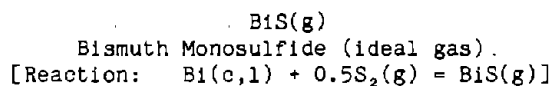
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 544.59 K, melting point of Bi; $\Delta H^\circ = 2.700$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-3000 K: $\text{Cp}^\circ = 8.745 + 0.294 \times 10^{-3}T - 0.353 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 8.745 \times 10^{-3}T + 0.147 \times 10^{-6}T^2 + 0.353 \times 10^{-2}T^{-1} - 2.739$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta \text{Hf}^\circ = 41.884 - 2.752 \times 10^{-3}T - 1.338 \times 10^{-6}T^2 - 43.200T^{-1}$
 $\Delta \text{Gf}^\circ = 41.884 + 2.752 \times 10^{-3}T \ln T + 1.338 \times 10^{-6}T^2 - 21.600T^{-1} - 59.851 \times 10^{-3}T$
 368.3-388.36 K: $\Delta \text{Hf}^\circ = 40.769 - 0.489 \times 10^{-3}T - 3.084 \times 10^{-6}T^2 + 112.400T^{-1}$
 $\Delta \text{Gf}^\circ = 40.769 + 0.489 \times 10^{-3}T \ln T + 3.084 \times 10^{-6}T^2 + 56.200T^{-1} - 44.668 \times 10^{-3}T$
 388.36-432.02 K: $\Delta \text{Hf}^\circ = 24.611 + 44.251 \times 10^{-3}T - 46.366 \times 10^{-6}T^2 + 2014.600T^{-1}$
 $\Delta \text{Gf}^\circ = 24.611 - 44.251 \times 10^{-3}T \ln T + 46.366 \times 10^{-6}T^2 + 1007.300T^{-1} + 240.561 \times 10^{-3}T$
 432.02-544.59 K: $\Delta \text{Hf}^\circ = 15.132 + 40.345 \times 10^{-3}T - 26.554 \times 10^{-6}T^2 + 5241.100T^{-1}$
 $\Delta \text{Gf}^\circ = 15.132 - 40.345 \times 10^{-3}T \ln T + 26.554 \times 10^{-6}T^2 + 2620.550T^{-1} + 238.713 \times 10^{-3}T$
 544.59-717.824 K: $\Delta \text{Hf}^\circ = 12.356 + 37.815 \times 10^{-3}T - 23.511 \times 10^{-6}T^2 + 5541.700T^{-1}$
 $\Delta \text{Gf}^\circ = 12.356 - 37.815 \times 10^{-3}T \ln T + 23.511 \times 10^{-6}T^2 + 2770.850T^{-1} + 229.023 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	8.436	61.599	61.599	0	25.445	19.248	-14.109
300	8.441	61.652	61.599	.016	25.443	19.211	-13.995
400	8.658	64.113	61.933	.872	25.279	17.155	-9.373
500	8.776	66.059	62.571	1.744	25.079	15.148	-6.621
544.59	8.808	66.810	62.888	2.136	24.973	14.264	-5.724
544.59	8.808	66.810	62.888	2.136	22.273	14.264	-5.724
600	8.847	67.666	63.291	2.625	22.128	13.454	-4.900
700	8.895	69.033	64.014	3.513	21.893	12.029	-3.756
800	8.931	70.224	64.719	4.404	21.670	10.638	-2.906
900	8.958	71.277	65.389	5.299	21.458	9.267	-2.250
1000	8.982	72.222	66.026	6.196	21.253	7.929	-1.733
1100	9.005	73.080	66.630	7.095	21.052	6.603	-1.312
1200	9.028	73.864	67.200	7.997	20.853	5.305	-.966
1300	9.053	74.588	67.741	8.901	20.652	4.016	-.675
1400	9.081	75.260	68.255	9.807	20.449	2.741	-.428
1500	9.112	75.887	68.742	10.717	20.247	1.486	-.217
1600	9.147	76.476	69.207	11.630	20.045	.243	-.033
1700	9.186	77.032	69.652	12.546	19.841	-.996	.128
1800	9.229	77.558	70.076	13.467	19.640	-2.218	.269
1837	9.246	77.746	70.229	13.809	19.567	-2.670	.318

Phase changes: 544.59 K, melting point of Bi; ΔH° = 2.700 kcal/mol.
1837 K, boiling point of Bi to equilibrium mixture of Bi(g) and Bi₂(g).

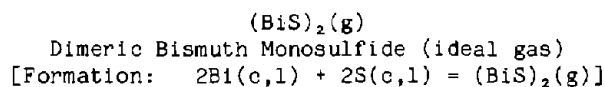
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $\text{Cp}^\circ = 8.745 + 0.294 \times 10^{-3}T - 0.353 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 8.745 \times 10^{-3}T + 0.147 \times 10^{-6}T^2 + 0.353 \times 10^{-2}T^{-1} - 2.739$

Reaction equations (kcal/mol):

298.15-544.59 K: $\Delta\text{Hr}^\circ = 25.096 + 1.250 \times 10^{-3}T - 3.215 \times 10^{-6}T^2 + 78.250T^{-1}$
 $\Delta\text{Gr}^\circ = 25.096 - 1.250 \times 10^{-3}T \ln T + 3.215 \times 10^{-6}T^2 + 39.125T^{-1} - 13.888 \times 10^{-3}T$
 544.59-1837 K: $\Delta\text{Hr}^\circ = 22.319 - 1.280 \times 10^{-3}T - 0.172 \times 10^{-6}T^2 + 378.850T^{-1}$
 $\Delta\text{Gr}^\circ = 22.319 + 1.280 \times 10^{-3}T \ln T + 0.172 \times 10^{-6}T^2 + 189.425T^{-1} - 23.578 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Cubicciotti (26), Prusaczyk (101), and Uy (121).
Other data based on Barrow (5-6).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	17.698	84.985	84.985	0	41.900	29.216	-21.415
300	17.719	85.095	84.985	.033	41.891	29.140	-21.228
368.3	18.278	88.798	85.359	1.266	41.515	26.271	-15.589
368.3	18.278	88.798	85.359	1.266	41.323	26.271	-15.589
388.36	18.443	89.772	85.563	1.635	41.200	25.456	-14.325
388.36	18.443	89.772	85.563	1.635	40.374	25.456	-14.325
400	18.538	90.318	85.693	1.850	40.266	25.010	-13.665
432.02	18.678	91.751	86.090	2.446	39.924	23.801	-12.040
500	18.976	94.506	87.050	3.728	38.954	21.348	-9.331
544.59	19.090	96.132	87.728	4.577	38.389	19.797	-7.945
544.59	19.090	96.132	87.728	4.577	32.989	19.797	-7.945
600	19.232	97.990	88.592	5.639	32.335	18.483	-6.732
700	19.394	100.968	90.152	7.571	31.281	16.262	-5.077
717.824	19.413	101.456	90.427	7.917	31.109	15.883	-4.836

*Data except enthalpy of formation at 298 K estimated.

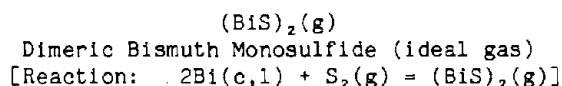
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 544.59 K, melting point of Bi; ΔH° = 2.700 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-3000 K: Cp° = 19.683 + 0.092x10⁻³T - 1.789x10⁻⁵T⁻²
 H° - H°₂₉₈ = 19.683x10⁻³T + 0.046x10⁻⁶T² + 1.789x10⁻²T⁻¹ - 6.473

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 43.074 - 3.311x10⁻³T - 2.924x10⁻⁶T² + 21.900T⁻¹
 ΔGf° = 43.074 + 3.311x10⁻³TlnT + 2.924x10⁻⁶T² + 10.950T⁻¹ - 66.339x10⁻³T
 368.3-388.36 K: ΔHf° = 40.843 + 1.215x10⁻³T - 6.416x10⁻⁶T² + 333.100T⁻¹
 ΔGf° = 40.843 - 1.215x10⁻³TlnT + 6.416x10⁻⁶T² + 166.550T⁻¹ - 35.973x10⁻³T
 388.36-432.02 K: ΔHf° = 8.527 + 90.695x10⁻³T - 92.980x10⁻⁶T² + 4137.500T⁻¹
 ΔGf° = 8.527 - 90.695x10⁻³TlnT + 92.980x10⁻⁶T² + 2068.750T⁻¹ + 534.484x10⁻³T
 432.02-544.59 K: ΔHf° = -10.431 + 82.883x10⁻³T - 53.356x10⁻⁶T² + 10590.500T⁻¹
 ΔGf° = -10.431 - 82.883x10⁻³TlnT + 53.356x10⁻⁶T² + 5295.250T⁻¹ + 530.789x10⁻³T
 544.59-717.824 K: ΔHf° = -15.984 + 77.823x10⁻³T - 47.270x10⁻⁶T² + 11191.700T⁻¹
 ΔGf° = -15.984 - 77.823x10⁻³TlnT + 47.270x10⁻⁶T² + 5595.850T⁻¹ + 511.408x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	17.698	84.985	84.985	0	11.190	10.189	-7.468
300	17.719	85.095	84.985	.033	11.187	10.185	-7.420
400	18.538	90.318	85.693	1.850	10.964	9.879	-5.397
500	18.976	94.506	87.050	3.728	10.699	9.642	-4.214
544.59	19.090	96.132	87.728	4.577	10.550	9.548	-3.832
544.59	19.090	96.132	87.728	4.577	5.150	9.548	-3.832
600	19.232	97.990	88.592	5.639	4.946	10.002	-3.643
700	19.394	100.968	90.152	7.571	4.631	10.872	-3.394
800	19.502	103.565	91.669	9.517	4.350	11.792	-3.221
900	19.577	105.867	93.121	11.471	4.090	12.726	-3.090
1000	19.632	107.932	94.501	13.431	3.845	13.710	-2.996
1100	19.673	109.806	95.809	15.397	3.610	14.702	-2.921
1200	19.704	111.519	97.047	17.366	3.377	15.732	-2.865
1300	19.729	113.097	98.222	19.337	3.139	16.770	-2.819
1400	19.748	114.560	99.338	21.311	2.896	17.823	-2.782
1500	19.764	115.923	100.398	23.287	2.648	18.902	-2.754
1600	19.777	117.199	101.409	25.264	2.394	19.996	-2.731
1700	19.788	118.398	102.373	27.242	2.133	21.090	-2.711
1800	19.797	119.529	103.295	29.221	1.868	22.208	-2.696
1837	19.800	119.932	103.626	29.954	1.769	22.620	-2.691

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 544.59 K, melting point of Bi; ΔH° = 2.700 kcal/mol.
 1837 K, boiling point of Bi to equilibrium mixture of Bi(g) and Bi₂(g).

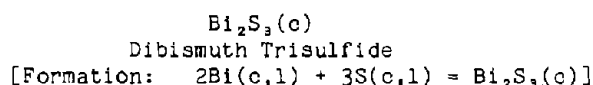
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: Cp° = 19.683 + 0.092x10⁻³T - 1.789x10⁻⁵T⁻²
 H° - H₂₉₈° = 19.683x10⁻³T + 0.046x10⁻⁶T² + 1.789x10⁻²T⁻¹ - 6.473

Reaction equations (kcal/mol):

298.15-544.59 K: ΔHr° = 9.496 + 4.694x10⁻³T - 6.678x10⁻⁶T² + 264.800T⁻¹
 ΔGr° = 9.496 - 4.694x10⁻³T lnT + 6.678x10⁻⁶T² + 132.400T⁻¹ + 25.587x10⁻³T
 544.59-1837 K: ΔHr° = 3.943 - 0.366x10⁻³T - 0.592x10⁻⁶T² + 866.000T⁻¹
 ΔGr° = 3.943 + 0.366x10⁻³T lnT + 0.592x10⁻⁶T² + 433.000T⁻¹ + 6.207x10⁻³T

Source: Data based on Prusaczyk (101) who estimated molecular constants.



T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	29.170	47.900	47.900	0	-43.000	-42.343	31.038
300*	29.203	48.081	47.901	.054	-42.998	-42.337	30.842
350	29.959	52.642	48.259	1.534	-42.968	-42.233	26.371
368.3	30.179	54.174	48.515	2.084	-42.962	-42.195	25.038
368.3	30.179	54.174	48.515	2.084	-43.250	-42.195	25.038
388.36	30.419	55.782	48.850	2.692	-43.251	-42.136	23.712
388.36	30.419	55.782	48.850	2.692	-44.490	-42.136	23.712
400	30.559	56.682	49.064	3.047	-44.547	-42.065	22.983
432.02	30.893	59.049	49.716	4.032	-44.763	-41.859	21.175
450	31.080	60.312	50.114	4.589	-45.104	-41.728	20.266
500	31.552	63.612	51.304	6.154	-45.567	-41.327	18.064
544.59	31.936	66.324	52.424	7.570	-45.961	-40.937	16.428
544.59	31.936	66.324	52.424	7.570	-51.361	-40.937	16.428
550	31.983	66.640	52.562	7.743	-51.387	-40.831	16.225
600	32.377	69.440	53.853	9.352	-51.756	-39.860	14.519
650	32.734	72.046	55.154	10.980	-52.039	-38.855	13.064
700	33.061	74.484	56.448	12.625	-52.269	-37.832	11.812
717.824	33.170	75.316	56.906	13.215	-52.334	-37.462	11.406

*Data above 298 K except temperature and enthalpy of fusion estimated.

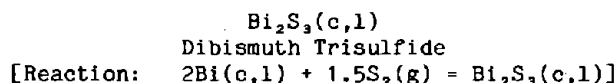
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 544.59 K, melting point of Bi; $\Delta H^\circ = 2.700$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-1036 K: $C_p^\circ = 29.620 + 5.344 \times 10^{-3}T - 1.815 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 29.620 \times 10^{-3}T + 2.672 \times 10^{-6}T^2 + 1.815 \times 10^{-2}T^{-1} - 9.677$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -42.225 - 1.548 \times 10^{-3}T + 1.419 \times 10^{-6}T^2 - 131.100T^{-1}$
 $\Delta G_f^\circ = -42.225 + 1.548 \times 10^{-3}T \ln T - 1.419 \times 10^{-6}T^2 - 65.550T^{-1} - 8.056 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -45.570 + 5.241 \times 10^{-3}T - 3.819 \times 10^{-6}T^2 + 335.700T^{-1}$
 $\Delta G_f^\circ = -45.570 - 5.241 \times 10^{-3}T \ln T + 3.819 \times 10^{-6}T^2 + 167.850T^{-1} + 37.493 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -94.045 + 139.461 \times 10^{-3}T - 133.665 \times 10^{-6}T^2 + 6042.300T^{-1}$
 $\Delta G_f^\circ = -94.045 - 139.461 \times 10^{-3}T \ln T + 133.665 \times 10^{-6}T^2 + 3021.150T^{-1} + 893.178 \times 10^{-3}T$
 432.02-544.59 K: $\Delta H_f^\circ = -122.481 + 127.743 \times 10^{-3}T - 74.229 \times 10^{-6}T^2 + 15721.800T^{-1}$
 $\Delta G_f^\circ = -122.481 - 127.743 \times 10^{-3}T \ln T + 74.229 \times 10^{-6}T^2 + 7860.900T^{-1} + 887.635 \times 10^{-3}T$
 544.59-717.824 K: $\Delta H_f^\circ = -128.035 + 122.683 \times 10^{-3}T - 68.143 \times 10^{-6}T^2 + 16323.000T^{-1}$
 $\Delta G_f^\circ = -128.035 - 122.683 \times 10^{-3}T \ln T + 68.143 \times 10^{-6}T^2 + 8161.500T^{-1} + 868.255 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	29.170	47.900	47.900	0	-89.065	-70.884	51.959
300*	29.203	48.081	47.901	.054	-89.054	-70.769	51.554
350	29.959	52.642	48.259	1.534	-88.780	-67.748	42.303
400	30.559	56.682	49.064	3.047	-88.500	-64.762	35.384
450	31.080	60.312	50.114	4.589	-88.217	-61.806	30.017
500	31.552	63.612	51.304	6.154	-87.950	-58.887	25.739
544.59	31.936	66.324	52.424	7.570	-87.719	-56.310	22.598
544.59	31.936	66.324	52.424	7.570	-93.119	-56.310	22.598
550	31.983	66.640	52.562	7.743	-93.095	-55.944	22.230
600	32.377	69.440	53.853	9.352	-92.840	-52.583	19.153
650	32.734	72.046	55.154	10.980	-92.551	-49.238	16.555
700	33.061	74.484	56.448	12.625	-92.244	-45.918	14.336
750	33.366	76.775	57.727	14.286	-91.915	-42.611	12.417
800	33.654	78.938	58.987	15.961	-91.571	-39.337	10.746
850	33.931	80.986	60.220	17.651	-91.209	-36.094	9.280
900	34.197	82.933	61.429	19.354	-90.832	-32.863	7.980
950	34.451	84.789	62.609	21.071	-90.439	-29.641	6.819
1000	34.703	86.563	63.764	22.799	-90.035	-26.452	5.781
1036	34.900	87.793	64.577	24.052	-89.735	-24.168	5.098
1036	50	106.104	64.577	43.022	-70.765	-24.168	5.098
1050	50	106.775	65.135	43.722	-70.436	-23.545	4.901
1100	50	109.101	67.081	46.222	-69.261	-21.340	4.240
1150	50	111.324	68.957	48.722	-68.085	-19.178	3.645
1200	50	113.452	70.767	51.222	-66.914	-17.077	3.110

*Data above 298 K estimated except temperature and enthalpy of fusion.

Phase changes: 544.59 K, melting point of Bi; ΔH° = 2.700 kcal/mol.
1036 K, melting point of Bi₂S₃; ΔH° = 18.970 kcal/mol.

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

298.15-1036 K: $C_p^\circ = 29.620 + 5.344 \times 10^{-3}T - 1.815 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 29.620 \times 10^{-3}T + 2.672 \times 10^{-6}T^2 + 1.815 \times 10^{-2}T^{-1} - 9.677$
 1036-1200 K: $C_p^\circ = 50.000$
 $H^\circ - H_{298}^\circ = 50.000 \times 10^{-3}T - 8.778$

Reaction equations (kcal/mol):

298.15-544.59 K: $\Delta H_r^\circ = -92.591 + 10.459 \times 10^{-3}T - 4.212 \times 10^{-6}T^2 + 233.250T^{-1}$
 $\Delta G_r^\circ = -92.591 - 10.459 \times 10^{-3}T \ln T + 4.212 \times 10^{-6}T^2 + 116.625T^{-1} + 129.833 \times 10^{-3}T$
 544.59-1036 K: $\Delta H_r^\circ = -98.145 + 5.399 \times 10^{-3}T + 1.874 \times 10^{-6}T^2 + 834.450T^{-1}$
 $\Delta G_r^\circ = -98.145 - 5.399 \times 10^{-3}T \ln T - 1.874 \times 10^{-6}T^2 + 417.225T^{-1} + 110.453 \times 10^{-3}T$
 1036-1200 K: $\Delta H_r^\circ = -97.245 + 25.779 \times 10^{-3}T - 0.798 \times 10^{-6}T^2 + 652.950T^{-1}$
 $\Delta G_r^\circ = -97.245 - 25.779 \times 10^{-3}T \ln T + 0.798 \times 10^{-6}T^2 + 326.475T^{-1} + 248.402 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Prusaczyk (101) and Mitchell (81). Low-temperature heat capacities and entropy at 298 K from Romanovskii (102). Fusion data from Glatz (44). All other data estimated.

$\text{Bi}_2\text{S}_3(\text{g})$
 Dibismuth Trisulfide (ideal gas)
 [Formation: $2\text{Bi}(\text{c,l}) + 3\text{S}(\text{c,l}) = \text{Bi}_2\text{S}_3(\text{g})$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHf°	ΔGf°	
298.15*	24.315	103.032	103.032	0	43.200	27.419	-20.099
300	24.331	103.183	103.033	.045	43.193	27.324	-19.905
368.3	24.750	108.225	103.541	1.725	42.879	23.738	-14.086
368.3	24.750	108.225	103.541	1.725	42.591	23.738	-14.086
388.36	24.873	109.541	103.817	2.223	42.480	22.717	-12.784
388.36	24.873	109.541	103.817	2.223	41.241	22.717	-12.784
400	24.944	110.277	103.994	2.513	41.119	22.163	-12.109
432.02	25.042	112.202	104.532	3.313	40.718	20.659	-10.451
500	25.250	115.880	105.832	5.024	39.503	17.609	-7.697
544.59	25.327	118.040	106.744	6.152	38.820	15.680	-6.292
544.59	25.327	118.040	106.744	6.152	33.420	15.680	-6.292
600	25.423	120.500	107.903	7.558	32.650	13.910	-5.067
700	25.529	124.428	109.991	10.106	31.412	10.888	-3.399
717.824	25.541	125.070	110.357	10.561	31.212	10.370	-3.157

*Data except enthalpy of formation at 298 K estimated.

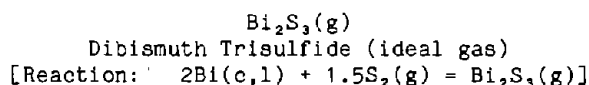
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta\text{H}^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta\text{H}^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta\text{H}^\circ = 0$ kcal/mol.
 544.59 K, melting point of Bi; $\Delta\text{H}^\circ = 2.700$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-3000 K: $\text{Cp}^\circ = 25.768 + 0.032 \times 10^{-3}T - 1.300 \times 10^{-5}T^{-2}$
 $\text{H}^\circ - \text{H}_{298}^\circ = 25.768 \times 10^{-3}T + 0.016 \times 10^{-6}T^2 + 1.300 \times 10^{-2}T^{-1} - 8.120$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta\text{Hf}^\circ = 45.532 - 5.400 \times 10^{-3}T - 1.237 \times 10^{-6}T^2 - 182.600T^{-1}$
 $\Delta\text{Gf}^\circ = 45.532 + 5.400 \times 10^{-3}T \ln T + 1.237 \times 10^{-6}T^2 - 91.300T^{-1} - 90.861 \times 10^{-3}T$
 368.3-388.36 K: $\Delta\text{Hf}^\circ = 42.187 + 1.389 \times 10^{-3}T - 6.475 \times 10^{-6}T^2 + 284.200T^{-1}$
 $\Delta\text{Gf}^\circ = 42.187 - 1.389 \times 10^{-3}T \ln T + 6.475 \times 10^{-6}T^2 + 142.100T^{-1} - 45.312 \times 10^{-3}T$
 388.36-432.02 K: $\Delta\text{Hf}^\circ = -6.288 + 135.609 \times 10^{-3}T - 136.321 \times 10^{-6}T^2 + 5990.800T^{-1}$
 $\Delta\text{Gf}^\circ = -6.288 - 135.609 \times 10^{-3}T \ln T + 136.321 \times 10^{-6}T^2 + 2995.400T^{-1} + 810.373 \times 10^{-3}T$
 432.02-544.59 K: $\Delta\text{Hf}^\circ = -34.724 + 123.891 \times 10^{-3}T - 76.885 \times 10^{-6}T^2 + 15670.300T^{-1}$
 $\Delta\text{Gf}^\circ = -34.724 - 123.891 \times 10^{-3}T \ln T + 76.885 \times 10^{-6}T^2 + 7835.150T^{-1} + 804.831 \times 10^{-3}T$
 544.59-717.824 K: $\Delta\text{Hf}^\circ = -40.277 + 118.831 \times 10^{-3}T - 70.799 \times 10^{-6}T^2 + 16271.500T^{-1}$
 $\Delta\text{Gf}^\circ = -40.277 - 118.831 \times 10^{-3}T \ln T + 70.799 \times 10^{-6}T^2 + 8135.750T^{-1} + 785.451 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHr°	ΔGr°	
298.15*	24.315	103.032	103.032	0	-2.865	-1.122	.822
300	24.331	103.183	103.033	.045	-2.863	-1.108	.807
400	24.944	110.277	103.994	2.513	-2.834	-.534	.292
500	25.250	115.880	105.832	5.024	-2.879	.049	-.021
544.59	25.327	118.040	106.744	6.152	-2.938	.307	-.123
544.59	25.327	118.040	106.744	6.152	-8.338	.307	-.123
600	25.423	120.500	107.903	7.558	-8.433	1.187	-.432
700	25.529	124.428	109.991	10.106	-8.563	2.803	-.875
800	25.599	127.842	112.013	12.663	-8.668	4.442	-1.214
900	25.648	130.860	113.942	15.226	-8.759	6.075	-1.475
1000	25.683	133.564	115.772	17.792	-8.842	7.740	-1.691
1100	25.709	136.013	117.502	20.362	-8.921	9.397	-1.867
1200	25.728	138.251	119.139	22.934	-9.002	11.076	-2.017
1300	25.744	140.311	120.690	25.507	-9.092	12.751	-2.144
1400	25.756	142.219	122.160	28.082	-9.192	14.431	-2.253
1500	25.766	143.996	123.557	30.658	-9.302	16.126	-2.350
1600	25.774	145.659	124.886	33.236	-9.421	17.829	-2.435
1700	25.781	147.222	126.156	35.813	-9.553	19.520	-2.509
1800	25.787	148.696	127.367	38.392	-9.689	21.230	-2.578
1837	25.788	149.221	127.802	39.346	-9.742	21.859	-2.601

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 544.59 K, melting point of Bi; $\Delta\text{H}^\circ = 2.700$ kcal/mol.
 1837 K, boiling point of Bi to equilibrium mixture of Bi(g) and Bi₂(g).

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

298.15-3000 K: $\text{Cp}^\circ = 25.768 + 0.032 \times 10^{-3}T - 1.300 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 25.768 \times 10^{-3}T + 0.016 \times 10^{-6}T^2 + 1.300 \times 10^{-2}T^{-1} - 8.120$

Reaction equations (kcal/mol):

298.15-544.59 K: $\Delta\text{Hr}^\circ = -4.834 + 6.607 \times 10^{-3}T - 6.868 \times 10^{-6}T^2 + 181.750T^{-1}$
 $\Delta\text{Gr}^\circ = -4.834 - 6.607 \times 10^{-3}T \ln T + 6.868 \times 10^{-6}T^2 + 90.875T^{-1} + 47.028 \times 10^{-3}T$
 544.59-1837 K: $\Delta\text{Hr}^\circ = -10.387 + 1.547 \times 10^{-3}T - 0.782 \times 10^{-6}T^2 + 782.950T^{-1}$
 $\Delta\text{Gr}^\circ = -10.387 - 1.547 \times 10^{-3}T \ln T + 0.782 \times 10^{-6}T^2 + 391.475T^{-1} + 27.648 \times 10^{-3}T$

Source: Data based on Prusaczyk (101) who estimated molecular constants.

COS(g)
Carbon Oxide Sulfide (ideal gas)
[Formation: $C(c) + 0.5O_2(g) + S(c,l) = COS(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	9.930	55.338	55.338	0	-33.870	-40.370	29.592
300	9.953	55.400	55.340	.018	-33.872	-40.411	29.439
368.3	10.640	57.518	55.551	.725	-33.950	-41.891	24.858
368.3	10.640	57.518	55.551	.725	-34.046	-41.891	24.858
388.36	10.842	58.088	55.667	.940	-34.074	-42.317	23.814
388.36	10.842	58.088	55.667	.940	-34.487	-42.317	23.814
400	10.959	58.410	55.743	1.067	-34.522	-42.552	23.249
432.02	11.188	59.263	55.972	1.422	-34.641	-43.190	21.849
500	11.675	60.936	56.534	2.201	-35.008	-44.504	19.452
600	12.227	63.115	57.453	3.397	-35.424	-46.362	16.887
700	12.669	65.034	58.403	4.642	-35.792	-48.156	15.035
717.824	12.733	65.353	58.571	4.868	-35.852	-48.470	14.757

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $C_p^\circ = 11.828 + 1.746 \times 10^{-3}T - 2.150 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 11.828 \times 10^{-3}T + 0.873 \times 10^{-6}T^2 + 2.150 \times 10^{-2}T^{-1} - 4.325$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -32.518 - 3.479 \times 10^{-3}T + 1.573 \times 10^{-6}T^2 - 135.500T^{-1}$
 $\Delta G_f^\circ = -32.518 + 3.479 \times 10^{-3}T \ln T - 1.573 \times 10^{-6}T^2 - 67.750T^{-1} - 44.928 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = -33.633 - 1.216 \times 10^{-3}T - 0.174 \times 10^{-6}T^2 + 20.100T^{-1}$
 $\Delta G_f^\circ = -33.633 + 1.216 \times 10^{-3}T \ln T + 0.174 \times 10^{-6}T^2 + 10.050T^{-1} - 29.745 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = -49.791 + 43.524 \times 10^{-3}T - 43.456 \times 10^{-6}T^2 + 1922.300T^{-1}$
 $\Delta G_f^\circ = -49.791 - 43.524 \times 10^{-3}T \ln T + 43.456 \times 10^{-6}T^2 + 961.150T^{-1} + 255.483 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = -59.270 + 39.618 \times 10^{-3}T - 23.644 \times 10^{-6}T^2 + 5148.800T^{-1}$
 $\Delta G_f^\circ = -59.270 - 39.618 \times 10^{-3}T \ln T + 23.644 \times 10^{-6}T^2 + 2574.400T^{-1} + 253.636 \times 10^{-3}T$

COS(g)
Carbon Oxide Sulfide (ideal gas)
[Reaction: $C(c) + 0.5O_2(g) + 0.5S_2(g) = COS(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	9.930	55.338	55.338	0	-49.225	-49.884	36.566
300	9.953	55.400	55.340	.018	-49.224	-49.888	36.343
400	10.959	58.410	55.743	1.067	-49.174	-50.117	27.382
500	11.675	60.936	56.534	2.201	-49.135	-50.357	22.011
600	12.227	63.115	57.453	3.397	-49.118	-50.603	18.432
700	12.669	65.034	58.403	4.642	-49.117	-50.851	15.876
800	13.029	66.750	59.340	5.928	-49.124	-51.098	13.959
900	13.324	68.303	60.252	7.246	-49.140	-51.346	12.468
1000	13.567	69.719	61.128	8.591	-49.159	-51.590	11.275
1100	13.770	71.022	61.969	9.958	-49.183	-51.821	10.296
1200	13.939	72.228	62.775	11.344	-49.210	-52.070	9.483
1300	14.081	73.349	63.545	12.745	-49.242	-52.308	8.794
1400	14.202	74.397	64.283	14.159	-49.277	-52.543	8.202
1500	14.306	75.381	64.991	15.585	-49.316	-52.775	7.689
1600	14.396	76.307	65.670	17.020	-49.359	-53.003	7.240
1700	14.474	77.182	66.321	18.463	-49.409	-53.231	6.843
1800	14.543	78.011	66.948	19.914	-49.461	-53.452	6.490
1900	14.604	78.799	67.551	21.372	-49.517	-53.672	6.174
2000	14.659	79.550	68.133	22.835	-49.580	-53.890	5.889

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

298.15-2000 K: $C_p^\circ = 11.828 + 1.746 \times 10^{-3}T - 2.150 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 11.828 \times 10^{-3}T + 0.873 \times 10^{-6}T^2 + 2.150 \times 10^{-2}T^{-1} - 4.325$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -49.307 + 0.523 \times 10^{-3}T - 0.305 \times 10^{-6}T^2 - 14.050T^{-1}$
 $\Delta G_r^\circ = -49.307 - 0.523 \times 10^{-3}T \ln T + 0.305 \times 10^{-6}T^2 - 7.025T^{-1} + 1.035 \times 10^{-3}T$

Source: Data from Gurvich (49).

CS(g)
Carbon Monosulfide (ideal gas)
[Formation: C(c) + S(c,l) = CS(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	7.122	50.300	50.300	0	68.500	56.196	-41.192
300	7.126	50.344	50.301	.013	68.499	56.120	-40.883
368.3	7.314	51.824	50.450	.506	68.449	53.306	-31.631
368.3	7.314	51.824	50.450	.506	68.353	53.306	-31.631
388.36	7.369	52.213	50.531	.653	68.328	52.488	-29.537
388.36	7.369	52.213	50.531	.653	67.915	52.488	-29.537
400	7.401	52.431	50.583	.739	67.881	52.025	-28.425
432.02	7.494	53.004	50.742	.977	67.763	50.760	-25.678
500	7.690	54.113	51.125	1.494	67.382	48.118	-21.032
600	7.938	55.538	51.745	2.276	66.930	44.309	-16.139
700	8.137	56.777	52.377	3.080	66.510	40.572	-12.667
717.824	8.165	56.982	52.489	3.225	66.439	39.913	-12.152

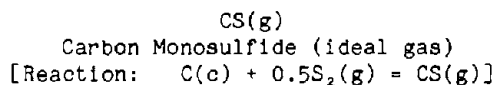
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-3000 K: Cp° = 7.990 + 0.476x10⁻³T - 0.898x10⁻⁵T²
 H°- H₂₉₈° = 7.990x10⁻³T + 0.238x10⁻⁶T² + 0.898x10⁻²T⁻¹ - 2.705

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 70.297 - 3.702x10⁻³T + 1.189x10⁻⁶T² - 238.100T⁻¹
 ΔGf° = 70.297 + 3.702x10⁻³TlnT - 1.189x10⁻⁶T² - 119.050T⁻¹ - 66.692x10⁻³T
 368.3-388.36 K: ΔHf° = 69.182 - 1.439x10⁻³T - 0.557x10⁻⁶T² - 82.500T⁻¹
 ΔGf° = 69.182 + 1.439x10⁻³TlnT + 0.557x10⁻⁶T² - 41.250T⁻¹ - 51.509x10⁻³T
 388.36-432.02 K: ΔHf° = 53.023 + 43.301x10⁻³T - 43.839x10⁻⁶T² + 1819.700T⁻¹
 ΔGf° = 53.023 - 43.301x10⁻³TlnT + 43.839x10⁻⁶T² + 909.850T⁻¹ + 233.720x10⁻³T
 432.02-717.824 K: ΔHf° = 43.545 + 39.395x10⁻³T - 24.027x10⁻⁶T² + 5046.200T⁻¹
 ΔGf° = 43.545 - 39.395x10⁻³TlnT + 24.027x10⁻⁶T² + 2523.100T⁻¹ + 231.872x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	7.122	50.300	50.300	0	53.145	46.683	-34.219
300	7.126	50.344	50.301	.013	53.147	46.643	-33.979
400	7.401	52.431	50.583	.739	53.230	44.460	-24.291
500	7.690	54.113	51.125	1.494	53.255	42.264	-18.473
600	7.938	55.538	51.745	2.276	53.236	40.068	-14.595
700	8.137	56.777	52.377	3.080	53.185	37.876	-11.825
800	8.293	57.875	52.998	3.902	53.112	35.694	-9.751
900	8.415	58.859	53.596	4.737	53.021	33.520	-8.140
1000	8.512	59.751	54.167	5.584	52.917	31.360	-6.854
1100	8.589	60.566	54.712	6.439	52.801	29.220	-5.805
1200	8.652	61.316	55.232	7.301	52.674	27.071	-4.930
1300	8.703	62.010	55.726	8.169	52.537	24.943	-4.193
1400	8.746	62.657	56.199	9.041	52.392	22.825	-3.563
1500	8.783	63.262	56.650	9.918	52.238	20.718	-3.019
1600	8.814	63.829	57.080	10.798	52.079	18.625	-2.544
1700	8.841	64.365	57.494	11.681	51.910	16.536	-2.126
1800	8.865	64.871	57.890	12.566	51.737	14.461	-1.756
1900	8.886	65.350	58.269	13.453	51.556	12.396	-1.426
2000	8.905	65.807	58.635	14.343	51.370	10.340	-1.130
2100	8.922	66.242	58.988	15.234	51.178	8.290	-.863
2200	8.937	66.657	59.327	16.127	50.981	6.254	-.621
2300	8.951	67.055	59.654	17.022	50.781	4.227	-.402
2400	8.965	67.436	59.970	17.918	50.573	2.206	-.201
2500	8.977	67.802	60.276	18.815	50.364	.196	-.017
2600	8.989	68.154	60.572	19.713	50.148	-1.806	.152
2700	9.000	68.494	60.860	20.612	49.930	-3.801	.308
2800	9.010	68.821	61.138	21.513	49.708	-5.786	.452
2900	9.021	69.138	61.409	22.414	49.483	-7.764	.585
3000	9.031	69.444	61.672	23.317	49.255	-9.736	.709

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

298.15-3000 K: $C_p^\circ = 7.990 + 0.476 \times 10^{-3}T - 0.898 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 7.990 \times 10^{-3}T + 0.238 \times 10^{-6}T^2 + 0.898 \times 10^{-2}T^{-1} - 2.705$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = 53.508 + 0.301 \times 10^{-3}T - 0.688 \times 10^{-6}T^2 - 116.650T^{-1}$
 $\Delta G_r^\circ = 53.508 - 0.301 \times 10^{-3}T \ln T + 0.688 \times 10^{-6}T^2 - 58.325T^{-1} - 20.729 \times 10^{-3}T$
2000-3000 K: $\Delta H_r^\circ = 56.525 - 2.406 \times 10^{-3}T + 0.054 \times 10^{-6}T^2 - 1260.200T^{-1}$
 $\Delta G_r^\circ = 56.525 + 2.406 \times 10^{-3}T \ln T - 0.054 \times 10^{-6}T^2 - 630.100T^{-1} - 41.182 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Bell (7) and Fincham (40). Other data based on Hildenbrand (53) and Lagerqvist (71).

CS₂(g)
Carbon Disulfide (ideal gas)
[Formation: C(c) + 2S(c,l) = CS₂(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	10.914	56.852	56.852	0	27.950	15.977	-11.711
300	10.935	56.919	56.852	.020	27.946	15.903	-11.585
368.3	11.576	59.234	57.083	.792	27.792	13.177	-7.819
368.3	11.576	59.234	57.083	.792	27.600	13.177	-7.819
388.36	11.764	59.853	57.210	1.026	27.543	12.394	-6.975
388.36	11.764	59.853	57.210	1.026	26.717	12.394	-6.975
400	11.873	60.202	57.292	1.164	26.646	11.966	-6.538
432.02	12.088	61.125	57.542	1.548	26.410	10.798	-5.463
500	12.546	62.927	58.155	2.386	25.677	8.404	-3.673
600	13.053	65.262	59.150	3.667	24.867	5.029	-1.832
700	13.442	67.305	60.172	4.993	24.169	1.778	-.555
717.824	13.496	67.644	60.353	5.233	24.056	1.211	-.369

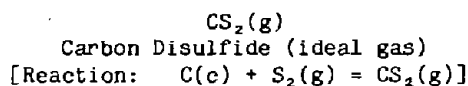
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-3000 K: Cp° = 13.332 + 0.870x10⁻³T - 2.380x10⁻⁵T²
H° - H₂₉₈° = 13.332x10⁻³T + 0.435x10⁻⁶T² + 2.380x10⁻²T⁻¹ - 4.812

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 30.446 - 6.534x10⁻³T + 3.103x10⁻⁶T² - 245.500T⁻¹
ΔGf° = 30.446 + 6.534x10⁻³T ln T - 3.103x10⁻⁶T² - 122.750T⁻¹ - 83.451x10⁻³T
368.3-388.36 K: ΔHf° = 28.215 - 2.008x10⁻³T - 0.389x10⁻⁶T² + 65.700T⁻¹
ΔGf° = 28.215 + 2.008x10⁻³T ln T + 0.389x10⁻⁶T² + 32.850T⁻¹ - 53.085x10⁻³T
388.36-432.02 K: ΔHf° = -4.101 + 87.472x10⁻³T - 86.953x10⁻⁶T² + 3870.100T⁻¹
ΔGf° = -4.101 - 87.472x10⁻³T ln T + 86.953x10⁻⁶T² + 1935.050T⁻¹ + 517.372x10⁻³T
432.02-717.824 K: ΔHf° = -23.059 + 79.660x10⁻³T - 47.329x10⁻⁶T² + 10323.100T⁻¹
ΔGf° = -23.059 - 79.660x10⁻³T ln T + 47.329x10⁻⁶T² + 5161.550T⁻¹ + 513.677x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	10.914	56.852	56.852	0	-2.760	-3.050	2.236
300	10.935	56.919	56.852	.020	-2.758	-3.052	2.223
400	11.873	60.202	57.292	1.164	-2.656	-3.166	1.730
500	12.546	62.927	58.155	2.386	-2.578	-3.302	1.444
600	13.053	65.262	59.150	3.667	-2.522	-3.453	1.258
700	13.442	67.305	60.172	4.993	-2.481	-3.612	1.128
800	13.743	69.120	61.179	6.353	-2.451	-3.774	1.031
900	13.980	70.753	62.154	7.739	-2.432	-3.944	.958
1000	14.169	72.236	63.089	9.147	-2.418	-4.112	.899
1100	14.322	73.594	63.983	10.572	-2.412	-4.271	.849
1200	14.448	74.846	64.837	12.011	-2.413	-4.451	.811
1300	14.553	76.006	65.651	13.461	-2.422	-4.620	.777
1400	14.643	77.088	66.430	14.921	-2.438	-4.789	.748
1500	14.720	78.101	67.175	16.389	-2.462	-4.957	.722
1600	14.787	79.053	67.888	17.864	-2.492	-5.121	.699
1700	14.846	79.952	68.572	19.346	-2.531	-5.287	.680
1800	14.899	80.802	69.228	20.834	-2.574	-5.445	.661
1900	14.947	81.609	69.858	22.326	-2.625	-5.604	.645
2000	14.991	82.376	70.465	23.823	-2.683	-5.757	.629
2100	15.031	83.109	71.050	25.324	-2.746	-5.913	.615
2200	15.068	83.809	71.614	26.829	-2.814	-6.061	.602
2300	15.103	84.479	72.159	28.337	-2.887	-6.204	.589
2400	15.135	85.123	72.686	29.849	-2.966	-6.350	.578
2500	15.166	85.741	73.195	31.364	-3.047	-6.487	.567
2600	15.195	86.337	73.690	32.882	-3.134	-6.626	.557
2700	15.222	86.911	74.169	34.403	-3.223	-6.757	.547
2800	15.249	87.465	74.634	35.927	-3.316	-6.886	.537
2900	15.275	88.000	75.085	37.453	-3.412	-7.008	.528
3000	15.299	88.519	75.525	38.982	-3.511	-7.135	.520

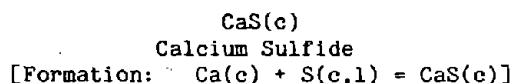
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $C_p^\circ = 13.332 + 0.870 \times 10^{-3}T - 2.380 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 13.332 \times 10^{-3}T + 0.435 \times 10^{-6}T^2 + 2.380 \times 10^{-2}T^{-1} - 4.812$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -3.132 + 1.471 \times 10^{-3}T - 0.651 \times 10^{-6}T^2 - 2.600T^{-1}$
 $\Delta G_r^\circ = -3.132 - 1.471 \times 10^{-3}T \ln T + 0.651 \times 10^{-6}T^2 - 1.300T^{-1} + 8.475 \times 10^{-3}T$
2000-3000 K: $\Delta H_r^\circ = 0.910 - 1.819 \times 10^{-3}T + 0.201 \times 10^{-6}T^2 - 1742.000T^{-1}$
 $\Delta G_r^\circ = 0.910 + 1.819 \times 10^{-3}T \ln T - 0.201 \times 10^{-6}T^2 - 871.000T^{-1} - 16.631 \times 10^{-3}T$

Source: Data from Chase (17).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	11.339	13.528	13.528	0	-113.100	-111.886	82.013
300*	11.340	13.598	13.528	.021	-113.100	-111.877	81.501
368.3	11.627	15.956	13.766	.806	-113.117	-111.598	66.221
368.3	11.627	15.956	13.766	.806	-113.213	-111.598	66.221
388.36	11.711	16.574	13.895	1.040	-113.223	-111.509	62.751
388.36	11.711	16.574	13.895	1.040	-113.636	-111.509	62.751
400	11.760	16.921	13.978	1.177	-113.660	-111.445	60.890
432.02	11.859	17.830	14.231	1.555	-113.748	-111.265	56.286
500	12.070	19.579	14.841	2.369	-114.048	-110.849	48.451
600	12.320	21.803	15.821	3.589	-114.369	-110.176	40.131
700	12.510	23.717	16.816	4.831	-114.659	-109.459	34.174
717.824	12.539	24.032	16.991	5.054	-114.710	-109.323	33.284

*Data above 298 K estimated.

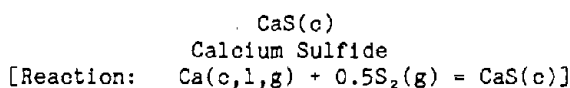
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: $C_p^\circ = 11.936 + 1.012 \times 10^{-3}T - 0.799 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 11.936 \times 10^{-3}T + 0.506 \times 10^{-6}T^2 + 0.799 \times 10^{-2}T^{-1} - 3.872$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -112.999 - 0.069 \times 10^{-3}T - 0.347 \times 10^{-6}T^2 - 14.700T^{-1}$
 $\Delta G_f^\circ = -112.999 + 0.069 \times 10^{-3}T \ln T + 0.347 \times 10^{-6}T^2 - 7.350T^{-1} + 3.321 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = -114.114 + 2.194 \times 10^{-3}T - 2.093 \times 10^{-6}T^2 + 140.900T^{-1}$
 $\Delta G_f^\circ = -114.114 - 2.194 \times 10^{-3}T \ln T + 2.093 \times 10^{-6}T^2 + 70.450T^{-1} + 18.504 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = -130.273 + 46.934 \times 10^{-3}T - 45.375 \times 10^{-6}T^2 + 2043.100T^{-1}$
 $\Delta G_f^\circ = -130.273 - 46.934 \times 10^{-3}T \ln T + 45.375 \times 10^{-6}T^2 + 1021.550T^{-1} + 303.733 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = -139.751 + 43.028 \times 10^{-3}T - 25.563 \times 10^{-6}T^2 + 5269.600T^{-1}$
 $\Delta G_f^\circ = -139.751 - 43.028 \times 10^{-3}T \ln T + 25.563 \times 10^{-6}T^2 + 2634.800T^{-1} + 301.885 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	11.339	13.528	13.528	0	-128.455	-121.399	88.987
300*	11.340	13.598	13.528	.021	-128.452	-121.354	88.405
400	11.760	16.921	13.978	1.177	-128.311	-119.010	65.023
500	12.070	19.579	14.841	2.369	-128.175	-116.702	51.010
600	12.320	21.803	15.821	3.589	-128.064	-114.417	41.676
700	12.510	23.717	16.816	4.831	-127.984	-112.154	35.016
720	12.542	24.070	17.012	5.082	-127.974	-111.698	33.905
720	12.542	24.070	17.012	5.082	-128.194	-111.698	33.905
800	12.670	25.398	17.786	6.090	-128.127	-109.866	30.014
900	12.800	26.898	18.717	7.363	-128.104	-107.572	26.122
1000	12.930	28.253	19.603	8.650	-128.208	-105.302	23.014
1100	13.046	29.491	20.446	9.949	-128.383	-103.002	20.464
1112	13.058	29.633	20.545	10.106	-128.411	-102.730	20.190
1112	13.058	29.633	20.545	10.106	-130.451	-102.730	20.190
1200	13.150	30.631	21.249	11.259	-130.311	-100.543	18.311
1300	13.239	31.687	22.012	12.578	-130.146	-98.070	16.487
1400	13.320	32.671	22.738	13.906	-129.977	-95.607	14.925
1500	13.381	33.592	23.431	15.241	-129.803	-93.162	13.574
1600	13.460	34.458	24.094	16.583	-129.627	-90.728	12.393
1700	13.566	35.277	24.727	17.935	-129.445	-88.292	11.351
1757	13.625	35.726	25.078	18.709	-129.338	-86.917	10.811
1757	13.625	35.726	25.078	18.709	-165.964	-86.917	10.811
1800	13.670	36.056	25.336	19.296	-165.796	-84.951	10.314
1900	13.774	36.798	25.920	20.669	-165.397	-80.470	9.256
2000	13.870	37.507	26.482	22.051	-164.993	-76.011	8.306

*Data above 298 K estimated.

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:

$$298.15-2000 \text{ K: } \text{Cp}^\circ = 11.936 + 1.012 \times 10^{-3}T - 0.799 \times 10^{-5}T^2$$

$$\text{H}^\circ - \text{H}^\circ_{298} = 11.936 \times 10^{-3}T + 0.506 \times 10^{-6}T^2 + 0.799 \times 10^{-2}T^{-1} - 3.872$$

Reaction equations (kcal/mol):

$$298.15-720 \text{ K: } \Delta \text{Hr}^\circ = -129.788 + 3.933 \times 10^{-3}T - 2.224 \times 10^{-6}T^2 + 106.750T^{-1}$$

$$\Delta \text{Gr}^\circ = -129.788 - 3.933 \times 10^{-3}T \ln T + 2.224 \times 10^{-6}T^2 + 53.375T^{-1} + 49.284 \times 10^{-3}T$$

$$720-1112 \text{ K: } \Delta \text{Hr}^\circ = -131.529 + 7.872 \times 10^{-3}T - 4.596 \times 10^{-6}T^2 + 45.750T^{-1}$$

$$\Delta \text{Gr}^\circ = -131.529 - 7.872 \times 10^{-3}T \ln T + 4.596 \times 10^{-6}T^2 + 22.875T^{-1} + 75.962 \times 10^{-3}T$$

$$1112-1757 \text{ K: } \Delta \text{Hr}^\circ = -131.777 + 0.764 \times 10^{-3}T + 0.346 \times 10^{-6}T^2 + 45.750T^{-1}$$

$$\Delta \text{Gr}^\circ = -131.777 - 0.764 \times 10^{-3}T \ln T - 0.346 \times 10^{-6}T^2 + 22.875T^{-1} + 31.833 \times 10^{-3}T$$

$$1757-2000 \text{ K: } \Delta \text{Hr}^\circ = -171.948 + 2.794 \times 10^{-3}T + 0.339 \times 10^{-6}T^2 + 45.750T^{-1}$$

$$\Delta \text{Gr}^\circ = -171.948 - 2.794 \times 10^{-3}T \ln T - 0.339 \times 10^{-6}T^2 + 22.875T^{-1} + 69.851 \times 10^{-3}T$$

Source: Data from Chase (17) who estimated all above 298 K.

CaS(g)
Calcium Sulfide (ideal gas)
[Formation: $\text{Ca(c)} + \text{S(c,l)} = \text{CaS(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	8.318	55.564	55.564	0	29.540	18.221	-13.356
300	8.325	55.615	55.565	.015	29.534	18.152	-13.224
368.3	8.499	57.344	55.738	.591	29.308	15.584	-9.247
368.3	8.499	57.344	55.738	.591	29.212	15.584	-9.247
388.36	8.550	57.796	55.833	.762	29.139	14.844	-8.354
388.36	8.550	57.796	55.833	.762	28.726	14.844	-8.354
400	8.580	58.049	55.894	.862	28.665	14.429	-7.884
432.02	8.625	58.711	56.079	1.137	28.475	13.296	-6.726
500	8.721	59.980	56.524	1.728	27.951	10.950	-4.786
600	8.807	61.578	57.238	2.604	27.286	7.614	-2.774
700	8.869	62.941	57.958	3.488	26.638	4.381	-1.368
717.824	8.879	63.164	58.085	3.646	26.522	3.819	-1.163

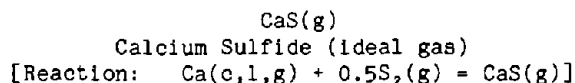
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2500 K: $C_p^\circ = 6.197 + 3.232 \times 10^{-3}T + 1.029 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 6.197 \times 10^{-3}T + 1.616 \times 10^{-6}T^2 - 1.029 \times 10^{-2}T^{-1} - 1.646$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 31.866 - 5.808 \times 10^{-3}T + 0.763 \times 10^{-6}T^2 - 197.500T^{-1}$
 $\Delta G_f^\circ = 31.866 + 5.808 \times 10^{-3}T \ln T - 0.763 \times 10^{-6}T^2 - 98.750T^{-1} - 77.519 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = 30.751 - 3.545 \times 10^{-3}T - 0.983 \times 10^{-6}T^2 - 41.900T^{-1}$
 $\Delta G_f^\circ = 30.751 + 3.545 \times 10^{-3}T \ln T + 0.983 \times 10^{-6}T^2 - 20.950T^{-1} - 62.336 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = 14.593 + 41.195 \times 10^{-3}T - 44.265 \times 10^{-6}T^2 + 1860.300T^{-1}$
 $\Delta G_f^\circ = 14.593 - 41.195 \times 10^{-3}T \ln T + 44.265 \times 10^{-6}T^2 + 930.150T^{-1} + 222.893 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = 5.114 + 37.289 \times 10^{-3}T - 24.453 \times 10^{-6}T^2 + 5086.800T^{-1}$
 $\Delta G_f^\circ = 5.114 - 37.289 \times 10^{-3}T \ln T + 24.453 \times 10^{-6}T^2 + 2543.400T^{-1} + 221.045 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	8.318	55.564	55.564	0	14.185	8.708	-6.383
300	8.325	55.615	55.565	.015	14.182	8.675	-6.319
400	8.580	58.049	55.894	.862	14.014	6.863	-3.750
500	8.721	59.980	56.524	1.728	13.824	5.096	-2.228
600	8.807	61.578	57.238	2.604	13.592	3.374	-1.229
700	8.869	62.941	57.958	3.488	13.313	1.686	-.526
720	8.880	63.191	58.100	3.665	13.250	1.358	-.412
720	8.880	63.191	58.100	3.665	13.030	1.358	-.412
800	8.924	64.129	58.656	4.378	12.801	.077	-.021
900	8.992	65.183	59.324	5.273	12.447	-1.478	.359
1000	9.097	66.136	59.959	6.177	11.959	-3.018	.660
1100	9.257	67.010	60.560	7.095	11.403	-4.487	.891
1112	9.285	67.111	60.630	7.206	11.330	-4.665	.917
1112	9.285	67.111	60.630	7.206	9.290	-4.665	.917
1200	9.489	67.825	61.132	8.031	9.102	-5.763	1.050
1300	9.801	68.596	61.677	8.995	8.911	-6.995	1.176
1400	10.192	69.336	62.197	9.994	8.751	-8.209	1.282
1500	10.651	70.055	62.698	11.036	8.632	-9.422	1.373
1600	11.163	70.758	63.179	12.126	8.556	-10.625	1.451
1700	11.704	71.451	63.646	13.269	8.530	-11.814	1.519
1757	12.016	71.843	63.906	13.945	8.538	-12.498	1.555
1757	12.016	71.843	63.906	13.945	-28.088	-12.498	1.555
1800	12.252	72.136	64.099	14.467	-27.985	-12.084	1.467
1900	12.781	72.812	64.539	15.719	-27.707	-11.206	1.289
2000	13.270	73.481	64.970	17.022	-27.383	-10.349	1.131

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.

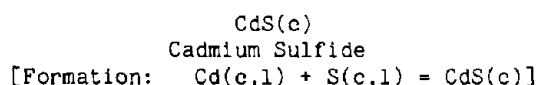
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $\text{Cp}^\circ = 6.197 + 3.232 \times 10^{-3}T + 1.029 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 6.197 \times 10^{-3}T + 1.616 \times 10^{-6}T^2 - 1.029 \times 10^{-2}T^{-1} - 1.646$

Reaction equations (kcal/mol):

298.15-720 K: $\Delta\text{Hr}^\circ = 15.077 - 1.806 \times 10^{-3}T - 1.114 \times 10^{-6}T^2 - 76.050T^{-1}$
 $\Delta\text{Gr}^\circ = 15.077 + 1.806 \times 10^{-3}T \ln T + 1.114 \times 10^{-6}T^2 - 38.025T^{-1} - 31.556 \times 10^{-3}T$
720-1112 K: $\Delta\text{Hr}^\circ = 13.336 + 2.133 \times 10^{-3}T - 3.486 \times 10^{-6}T^2 - 137.050T^{-1}$
 $\Delta\text{Gr}^\circ = 13.336 - 2.133 \times 10^{-3}T \ln T + 3.486 \times 10^{-6}T^2 - 68.525T^{-1} - 4.877 \times 10^{-3}T$
1112-1757 K: $\Delta\text{Hr}^\circ = 13.088 - 4.975 \times 10^{-3}T + 1.456 \times 10^{-6}T^2 - 137.050T^{-1}$
 $\Delta\text{Gr}^\circ = 13.088 + 4.975 \times 10^{-3}T \ln T - 1.456 \times 10^{-6}T^2 - 68.525T^{-1} - 49.007 \times 10^{-3}T$
1757-2000 K: $\Delta\text{Hr}^\circ = -27.083 - 2.945 \times 10^{-3}T + 1.449 \times 10^{-6}T^2 - 137.050T^{-1}$
 $\Delta\text{Gr}^\circ = -27.083 + 2.945 \times 10^{-3}T \ln T - 1.449 \times 10^{-6}T^2 - 68.525T^{-1} - 10.989 \times 10^{-3}T$

Source: Data from Chase (17) who estimated some molecular constants.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	11.303	17.252	17.252	0	-35.700	-34.868	25.559
300	11.316	17.322	17.252	.021	-35.700	-34.862	25.397
368.3	11.664	19.695	17.491	.812	-35.724	-34.671	20.574
368.3	11.664	19.695	17.491	.812	-35.820	-34.671	20.574
388.36	11.766	20.317	17.621	1.047	-35.833	-34.608	19.475
388.36	11.766	20.317	17.621	1.047	-36.246	-34.608	19.475
400	11.825	20.665	17.705	1.184	-36.272	-34.558	18.882
432.02	11.918	21.579	17.959	1.564	-36.364	-34.418	17.411
500	12.115	23.336	18.574	2.381	-36.676	-34.085	14.899
594.26	12.337	25.447	19.500	3.534	-36.983	-33.568	12.345
594.26	12.337	25.447	19.500	3.534	-38.463	-33.568	12.345
600	12.350	25.566	19.558	3.605	-38.482	-33.516	12.208
700	12.559	27.486	20.556	4.851	-38.746	-32.670	10.200
717.824	12.594	27.802	20.732	5.075	-38.785	-32.514	9.899

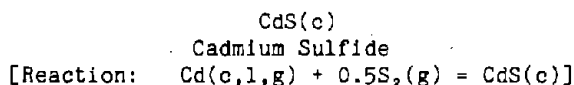
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 594.26 K, melting point of Cd; $\Delta H^\circ = 1.480$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-1100 K: $\text{Cp}^\circ = 11.693 + 1.476 \times 10^{-3}T - 0.738 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 11.693 \times 10^{-3}T + 0.738 \times 10^{-6}T^2 + 0.738 \times 10^{-2}T^{-1} - 3.799$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta \text{Hf}^\circ = -34.984 - 1.800 \times 10^{-3}T + 1.009 \times 10^{-6}T^2 - 80.200T^{-1}$
 $\Delta \text{Gf}^\circ = -34.984 + 1.800 \times 10^{-3}T \ln T - 1.009 \times 10^{-6}T^2 - 40.100T^{-1} - 9.116 \times 10^{-3}T$
 368.3-388.36 K: $\Delta \text{Hf}^\circ = -36.099 + 0.463 \times 10^{-3}T - 0.737 \times 10^{-6}T^2 + 75.400T^{-1}$
 $\Delta \text{Gf}^\circ = -36.099 - 0.463 \times 10^{-3}T \ln T + 0.737 \times 10^{-6}T^2 + 37.700T^{-1} + 6.067 \times 10^{-3}T$
 388.36-432.02 K: $\Delta \text{Hf}^\circ = -52.257 + 45.203 \times 10^{-3}T - 44.019 \times 10^{-6}T^2 + 1977.600T^{-1}$
 $\Delta \text{Gf}^\circ = -52.257 - 45.203 \times 10^{-3}T \ln T + 44.019 \times 10^{-6}T^2 + 988.800T^{-1} + 291.295 \times 10^{-3}T$
 432.02-594.26 K: $\Delta \text{Hf}^\circ = -61.736 + 41.297 \times 10^{-3}T - 24.207 \times 10^{-6}T^2 + 5204.100T^{-1}$
 $\Delta \text{Gf}^\circ = -61.736 - 41.297 \times 10^{-3}T \ln T + 24.207 \times 10^{-6}T^2 + 2602.050T^{-1} + 289.448 \times 10^{-3}T$
 594.26-717.824 K: $\Delta \text{Hf}^\circ = -62.663 + 39.511 \times 10^{-3}T - 22.761 \times 10^{-6}T^2 + 5202.500T^{-1}$
 $\Delta \text{Gf}^\circ = -62.663 - 39.511 \times 10^{-3}T \ln T + 22.761 \times 10^{-6}T^2 + 2601.250T^{-1} + 280.461 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	11.303	17.252	17.252	0	-51.055	-44.382	32.533
300	11.316	17.322	17.252	.021	-51.052	-44.339	32.301
400	11.825	20.665	17.705	1.184	-50.923	-42.124	23.015
500	12.115	23.336	18.574	2.381	-50.804	-39.939	17.457
594.26	12.337	25.447	19.500	3.534	-50.700	-37.900	13.938
594.26	12.337	25.447	19.500	3.534	-52.180	-37.900	13.938
600	12.350	25.566	19.558	3.605	-52.177	-37.757	13.753
700	12.559	27.486	20.556	4.851	-52.071	-35.365	11.041
800	12.754	29.176	21.531	6.116	-51.952	-32.986	9.011
900	12.941	30.689	22.458	7.408	-51.810	-30.613	7.434
1000	13.124	32.062	23.357	8.705	-51.666	-28.270	6.178
1040	13.195	32.578	23.702	9.231	-51.602	-27.344	5.746
1040	13.195	32.578	23.702	9.231	-75.411	-27.344	5.746
1100	13.302	33.321	24.206	10.026	-75.183	-24.577	4.883

Phase changes: 594.26 K, melting point of Cd; ΔH° = 1.480 kcal/mol.

1040 K, boiling point of Cd; ΔH° = 23.809 kcal/mol.

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

298.15-1100 K: $\text{Cp}^\circ = 11.693 + 1.476 \times 10^{-3}T - 0.738 \times 10^{-5}T^2$

$\text{H}^\circ - \text{H}_{298}^\circ = 11.693 \times 10^{-3}T + 0.738 \times 10^{-6}T^2 + 0.738 \times 10^{-2}T^{-1} - 3.799$

Reaction equations (kcal/mol):

298.15-594.26 K: $\Delta\text{Hr}^\circ = -51.773 + 2.202 \times 10^{-3}T - 0.868 \times 10^{-6}T^2 + 41.250T^{-1}$

$\Delta\text{Gr}^\circ = -51.773 - 2.202 \times 10^{-3}T \ln T + 0.868 \times 10^{-6}T^2 + 20.625T^{-1} + 36.847 \times 10^{-3}T$

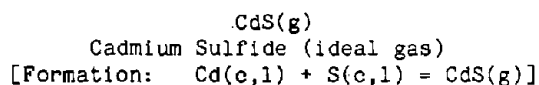
594.26-1040 K: $\Delta\text{Hr}^\circ = -52.699 + 0.416 \times 10^{-3}T + 0.578 \times 10^{-6}T^2 + 39.650T^{-1}$

$\Delta\text{Gr}^\circ = -52.699 - 0.416 \times 10^{-3}T \ln T - 0.578 \times 10^{-6}T^2 + 19.825T^{-1} + 27.860 \times 10^{-3}T$

1040-1100 K: $\Delta\text{Hr}^\circ = -78.731 + 2.553 \times 10^{-3}T + 0.578 \times 10^{-6}T^2 + 39.650T^{-1}$

$\Delta\text{Gr}^\circ = -78.731 - 2.553 \times 10^{-3}T \ln T - 0.578 \times 10^{-6}T^2 + 19.825T^{-1} + 67.736 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Adami (1). All other data from Beyer (9).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	8.600	58.930	58.930	0	45.000	33.405	-24.486
300	8.605	58.983	58.930	.016	44.995	33.335	-24.284
368.3	8.719	60.762	59.109	.609	44.773	30.701	-18.218
368.3	8.719	60.762	59.109	.609	44.677	30.701	-18.218
388.36	8.753	61.225	59.206	.784	44.604	29.942	-16.850
388.36	8.753	61.225	59.206	.784	44.191	29.942	-16.850
400	8.772	61.484	59.269	.886	44.130	29.516	-16.127
432.02	8.801	62.161	59.459	1.167	43.939	28.353	-14.343
500	8.863	63.452	59.916	1.768	43.411	25.944	-11.340
594.26	8.917	64.987	60.602	2.606	42.789	22.706	-8.350
594.26	8.917	64.987	60.602	2.606	41.309	22.706	-8.350
600	8.920	65.073	60.645	2.657	41.270	22.531	-8.207
700	8.960	66.451	61.378	3.551	40.654	19.455	-6.074
717.824	8.966	66.676	61.507	3.711	40.550	18.917	-5.759

*Data except enthalpy of formation at 298 K estimated.

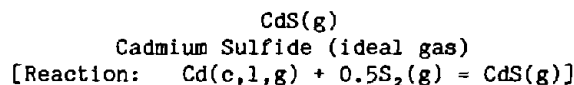
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 594.26 K, melting point of Cd; $\Delta H^\circ = 1.480$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-3000 K: $C_p^\circ = 8.928 + 0.142 \times 10^{-3}T - 0.329 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 8.928 \times 10^{-3}T + 0.071 \times 10^{-6}T^2 + 0.329 \times 10^{-2}T^{-1} - 2.779$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 46.737 - 4.565 \times 10^{-3}T + 0.342 \times 10^{-6}T^2 - 121.100T^{-1}$
 $\Delta G_f^\circ = 46.737 + 4.565 \times 10^{-3}T \ln T - 0.342 \times 10^{-6}T^2 - 60.550T^{-1} - 69.941 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = 45.622 - 2.302 \times 10^{-3}T - 1.404 \times 10^{-6}T^2 + 34.500T^{-1}$
 $\Delta G_f^\circ = 45.622 + 2.302 \times 10^{-3}T \ln T + 1.404 \times 10^{-6}T^2 + 17.250T^{-1} - 54.758 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = 29.463 + 42.438 \times 10^{-3}T - 44.686 \times 10^{-6}T^2 + 1936.700T^{-1}$
 $\Delta G_f^\circ = 29.463 - 42.438 \times 10^{-3}T \ln T + 44.686 \times 10^{-6}T^2 + 968.350T^{-1} + 230.471 \times 10^{-3}T$
 432.02-594.26 K: $\Delta H_f^\circ = 19.985 + 38.532 \times 10^{-3}T - 24.874 \times 10^{-6}T^2 + 5163.200T^{-1}$
 $\Delta G_f^\circ = 19.985 - 38.532 \times 10^{-3}T \ln T + 24.874 \times 10^{-6}T^2 + 2581.600T^{-1} + 228.623 \times 10^{-3}T$
 594.26-717.824 K: $\Delta H_f^\circ = 19.058 + 36.746 \times 10^{-3}T - 23.428 \times 10^{-6}T^2 + 5161.600T^{-1}$
 $\Delta G_f^\circ = 19.058 - 36.746 \times 10^{-3}T \ln T + 23.428 \times 10^{-6}T^2 + 2580.800T^{-1} + 219.636 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15*	8.600	58.930	58.930	0	29.645	23.892	-17.513
300	8.605	58.983	58.930	.016	29.643	23.857	-17.380
400	8.772	61.484	59.269	.886	29.479	21.950	-11.993
500	8.863	63.452	59.916	1.768	29.284	20.090	-8.781
594.26	8.917	64.987	60.602	2.606	29.072	18.375	-6.758
594.26	8.917	64.987	60.602	2.606	27.592	18.375	-6.758
600	8.920	65.073	60.645	2.657	27.576	18.291	-6.662
700	8.960	66.451	61.378	3.551	27.329	16.759	-5.232
800	8.991	67.650	62.089	4.449	27.082	15.268	-4.171
900	9.017	68.711	62.768	5.349	26.831	13.809	-3.353
1000	9.040	69.662	63.410	6.252	26.581	12.377	-2.705
1040	9.048	70.017	63.657	6.614	26.480	11.803	-2.480
1040	9.048	70.017	63.657	6.614	2.671	11.803	-2.480
1100	9.060	70.524	64.018	7.157	2.649	12.331	-2.450
1200	9.078	71.313	64.593	8.064	2.607	13.213	-2.406
1300	9.096	72.041	65.139	8.973	2.565	14.097	-2.370
1400	9.112	72.715	65.656	9.883	2.520	14.987	-2.339
1500	9.128	73.345	66.148	10.795	2.472	15.877	-2.313
1600	9.144	73.934	66.616	11.709	2.425	16.774	-2.291
1700	9.159	74.489	67.063	12.624	2.374	17.673	-2.272
1800	9.174	75.013	67.490	13.541	2.321	18.575	-2.255
1900	9.189	75.509	67.899	14.459	2.267	19.478	-2.240
2000	9.203	75.981	68.292	15.378	2.210	20.384	-2.227

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 594.26 K, melting point of Cd; $\Delta H^\circ = 1.480$ kcal/mol.
1040 K, boiling point of Cd; $\Delta H^\circ = 23.809$ kcal/mol.

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

298.15-3000 K: $C_p^\circ = 8.928 + 0.142 \times 10^{-3}T - 0.329 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 8.928 \times 10^{-3}T + 0.071 \times 10^{-6}T^2 + 0.329 \times 10^{-2}T^{-1} - 2.779$

Reaction equations (kcal/mol):

298.15-594.26 K: $\Delta H_r^\circ = 29.948 - 0.563 \times 10^{-3}T - 1.535 \times 10^{-6}T^2 + 0.350T^{-1}$
 $\Delta G_r^\circ = 29.948 + 0.563 \times 10^{-3}T \ln T + 1.535 \times 10^{-6}T^2 + 0.175T^{-1} - 23.978 \times 10^{-3}T$
594.26-1040 K: $\Delta H_r^\circ = 29.021 - 2.349 \times 10^{-3}T - 0.089 \times 10^{-6}T^2 - 1.250T^{-1}$
 $\Delta G_r^\circ = 29.021 + 2.349 \times 10^{-3}T \ln T + 0.089 \times 10^{-6}T^2 - 0.625T^{-1} - 32.965 \times 10^{-3}T$
1040-2000 K: $\Delta H_r^\circ = 2.990 - 0.212 \times 10^{-3}T - 0.089 \times 10^{-6}T^2 - 1.250T^{-1}$
 $\Delta G_r^\circ = 2.990 + 0.212 \times 10^{-3}T \ln T + 0.089 \times 10^{-6}T^2 - 0.625T^{-1} + 6.911 \times 10^{-3}T$

Source: Data based on Marquart (77) who estimated molecular constants.

CeS(c)
Cerium Monosulfide
[Formation: $\text{Ce(c)} + \text{S(c,1)} = \text{CeS(c)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	11.940	18.670	18.670	0	-109.800	-107.954	79.132
300	11.951	18.744	18.671	.022	-109.800	-107.943	78.635
368.3	12.366	21.235	18.922	.852	-109.801	-107.519	63.801
368.3	12.366	21.235	18.922	.852	-109.897	-107.519	63.801
388.36	12.488	21.894	19.059	1.101	-109.901	-107.389	60.432
388.36	12.488	21.894	19.059	1.101	-110.314	-107.389	60.432
400	12.559	22.264	19.146	1.247	-110.335	-107.301	58.626
432.02	12.763	23.239	19.414	1.652	-110.411	-107.056	54.157
500	13.197	25.135	20.065	2.535	-110.677	-106.506	46.553
600	13.846	27.598	21.120	3.887	-110.909	-105.645	38.481
700	14.502	29.782	22.205	5.304	-111.056	-104.760	32.707
717.824	14.619	30.148	22.398	5.563	-111.074	-104.599	31.846

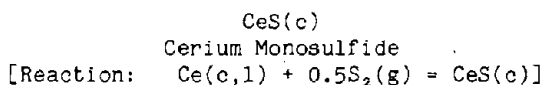
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $C_p^\circ = 9.825 + 6.646 \times 10^{-3}T + 0.121 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 9.825 \times 10^{-3}T + 3.323 \times 10^{-6}T^2 - 0.121 \times 10^{-2}T^{-1} - 3.184$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -108.546 - 3.434 \times 10^{-3}T + 3.093 \times 10^{-6}T^2 - 150.500T^{-1}$
 $\Delta G_f^\circ = -108.546 + 3.434 \times 10^{-3}T \ln T - 3.093 \times 10^{-6}T^2 - 75.250T^{-1} - 15.811 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -109.661 - 1.171 \times 10^{-3}T + 1.347 \times 10^{-6}T^2 + 5.100T^{-1}$
 $\Delta G_f^\circ = -109.661 + 1.171 \times 10^{-3}T \ln T - 1.347 \times 10^{-6}T^2 + 2.550T^{-1} - 0.628 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -125.820 + 43.569 \times 10^{-3}T - 41.935 \times 10^{-6}T^2 + 1907.300T^{-1}$
 $\Delta G_f^\circ = -125.820 - 43.569 \times 10^{-3}T \ln T + 41.935 \times 10^{-6}T^2 + 953.650T^{-1} + 284.601 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -135.298 + 39.663 \times 10^{-3}T - 22.123 \times 10^{-6}T^2 + 5133.800T^{-1}$
 $\Delta G_f^\circ = -135.298 - 39.663 \times 10^{-3}T \ln T + 22.123 \times 10^{-6}T^2 + 2566.900T^{-1} + 282.753 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	11.940	18.670	18.670	0	-125.155	-117.468	86.105
300	11.951	18.744	18.671	.022	-125.152	-117.420	85.539
400	12.559	22.264	19.146	1.247	-124.986	-114.867	62.759
500	13.197	25.135	20.065	2.535	-124.804	-112.359	49.112
600	13.846	27.598	21.120	3.887	-124.604	-109.885	40.025
700	14.502	29.782	22.205	5.304	-124.381	-107.455	33.549
800	15.161	31.762	23.277	6.788	-124.136	-105.046	28.697
900	15.822	33.585	24.322	8.337	-123.870	-102.678	24.933
999	16.476	35.271	25.325	9.936	-123.583	-100.366	21.957
999	16.476	35.271	25.325	9.936	-124.298	-100.366	21.957
1000	16.483	35.287	25.335	9.952	-124.295	-100.344	21.930
1071	16.954	36.433	26.033	11.139	-124.064	-98.647	20.130
1071	16.954	36.433	26.033	11.139	-125.369	-98.647	20.130
1100	17.146	36.889	26.314	11.633	-125.266	-97.924	19.455
1200*	17.809	38.409	27.258	13.381	-124.870	-95.459	17.385
1300	18.472	39.861	28.173	15.195	-124.411	-93.029	15.639
1400	19.136	41.254	29.057	17.076	-123.890	-90.630	14.148
1500	19.800	42.597	29.916	19.022	-123.307	-88.278	12.862
1600	20.464	43.896	30.749	21.035	-122.660	-85.966	11.742
1700	21.128	45.156	31.559	23.115	-121.951	-83.686	10.758
1800	21.792	46.383	32.349	25.261	-121.178	-81.467	9.891
1900	22.456	47.579	33.120	27.473	-120.342	-79.278	9.119
2000	23.120	48.747	33.871	29.752	-119.443	-77.143	8.430

*Data extrapolated above 1100 K.

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.

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

298.15-2000 K: $\text{Cp}^\circ = 9.825 + 6.646 \times 10^{-3}T + 0.121 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 9.825 \times 10^{-3}T + 3.323 \times 10^{-6}T^2 - 0.121 \times 10^{-2}T^{-1} - 3.184$

Reaction equations (kcal/mol):

298.15-999 K: $\Delta\text{Hr}^\circ = -125.335 + 0.568 \times 10^{-3}T + 1.216 \times 10^{-6}T^2 - 29.050T^{-1}$
 $\Delta\text{Gr}^\circ = -125.335 - 0.568 \times 10^{-3}T \ln T - 1.216 \times 10^{-6}T^2 - 14.525T^{-1} + 30.152 \times 10^{-3}T$
999-1071 K: $\Delta\text{Hr}^\circ = -124.075 - 3.337 \times 10^{-3}T + 3.163 \times 10^{-6}T^2 - 46.250T^{-1}$
 $\Delta\text{Gr}^\circ = -124.075 + 3.337 \times 10^{-3}T \ln T - 3.163 \times 10^{-6}T^2 - 23.125T^{-1} + 3.874 \times 10^{-3}T$
1071-2000 K: $\Delta\text{Hr}^\circ = -125.359 - 3.357 \times 10^{-3}T + 3.163 \times 10^{-6}T^2 - 46.250T^{-1}$
 $\Delta\text{Gr}^\circ = -125.359 + 3.357 \times 10^{-3}T \ln T - 3.163 \times 10^{-6}T^2 - 23.125T^{-1} + 4.933 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (104). Low-temperature heat capacities and entropy at 298 K from King (66). High-temperature data based on Mezaki (79). Data extrapolated above 1100 K.

CeS(g)
Cerium Monosulfide (ideal gas)
[Formation: $\text{Ce(c)} + \text{S(c,l)} = \text{CeS(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15*	8.180	62.030	62.030	0	31.400	20.318	-14.893
300	8.190	62.080	62.030	.015	31.393	20.249	-14.752
368.3	8.402	63.792	62.206	.584	31.131	17.739	-10.526
368.3	8.402	63.792	62.206	.584	31.035	17.739	-10.526
388.36	8.464	64.240	62.300	.753	30.951	17.018	-9.577
388.36	8.464	64.240	62.300	.753	30.538	17.018	-9.577
400	8.500	64.490	62.360	.852	30.470	16.614	-9.077
432.02	8.545	65.146	62.542	1.125	30.262	15.512	-7.847
500	8.640	66.400	62.980	1.710	29.698	13.236	-5.786
600	8.720	67.980	63.683	2.578	28.982	10.017	-3.649
700	8.770	69.330	64.397	3.453	28.293	6.905	-2.156
717.824	8.775	69.551	64.522	3.609	28.172	6.363	-1.937

*Data except enthalpy of formation at 298 K estimated.

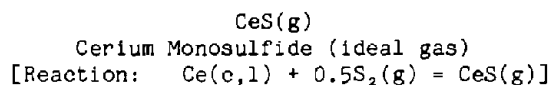
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $C_p^\circ = 8.873 + 0.036 \times 10^{-3}T - 0.626 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 8.873 \times 10^{-3}T + 0.018 \times 10^{-6}T^2 + 0.626 \times 10^{-3}T^3 - 2.857$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 32.981 - 4.386 \times 10^{-3}T - 0.212 \times 10^{-6}T^2 - 75.800T^{-1}$
 $\Delta G_f^\circ = 32.981 + 4.386 \times 10^{-3}T \ln T + 0.212 \times 10^{-6}T^2 - 37.900T^{-1} - 67.097 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = 31.866 - 2.123 \times 10^{-3}T - 1.958 \times 10^{-6}T^2 + 79.800T^{-1}$
 $\Delta G_f^\circ = 31.866 + 2.123 \times 10^{-3}T \ln T + 1.958 \times 10^{-6}T^2 + 39.900T^{-1} - 51.914 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = 15.707 + 42.617 \times 10^{-3}T - 45.240 \times 10^{-6}T^2 + 1982.000T^{-1}$
 $\Delta G_f^\circ = 15.707 - 42.617 \times 10^{-3}T \ln T + 45.240 \times 10^{-6}T^2 + 991.000T^{-1} + 233.314 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = 6.229 + 38.711 \times 10^{-3}T - 25.428 \times 10^{-6}T^2 + 5208.500T^{-1}$
 $\Delta G_f^\circ = 6.229 - 38.711 \times 10^{-3}T \ln T + 25.428 \times 10^{-6}T^2 + 2604.250T^{-1} + 231.466 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15*	8.180	62.030	62.030	0	16.045	10.804	-7.920
300	8.190	62.080	62.030	.015	16.041	10.772	-7.847
400	8.500	64.490	62.360	.852	15.819	9.048	-4.944
500	8.640	66.400	62.980	1.710	15.571	7.383	-3.227
600	8.720	67.980	63.683	2.578	15.288	5.776	-2.104
700	8.770	69.330	64.397	3.453	14.968	4.210	-1.314
800	8.800	70.510	65.096	4.331	14.607	2.698	-.737
900	8.830	71.540	65.748	5.213	14.206	1.238	-.301
999	8.850	72.471	66.377	6.088	13.770	-.176	.039
999	8.850	72.471	66.377	6.088	13.055	-.176	.039
1000	8.850	72.480	66.383	6.097	13.050	-.192	.042
1071	8.857	73.083	66.804	6.725	12.723	-1.112	.227
1071	8.857	73.083	66.804	6.725	11.418	-1.112	.227
1100	8.860	73.320	66.973	6.982	11.283	-1.449	.288
1200	8.870	74.090	67.532	7.869	10.819	-2.588	.471
1300	8.880	74.800	68.065	8.756	10.350	-3.689	.620
1400	8.890	75.460	68.571	9.645	9.880	-4.749	.741
1500	8.900	76.070	69.047	10.535	9.407	-5.774	.841
1600	8.910	76.650	69.509	11.425	8.930	-6.782	.926
1700	8.910	77.190	69.945	12.316	8.451	-7.743	.995
1800	8.920	77.700	70.363	13.207	7.968	-8.691	1.055
1900	8.920	78.180	70.759	14.100	7.485	-9.593	1.103
2000	8.930	78.640	71.144	14.992	6.997	-10.488	1.146

*Data except enthalpy of formation at 298 K estimated.

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.

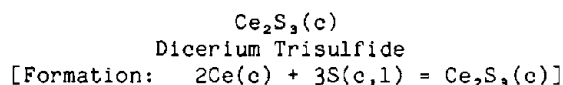
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 8.873 + 0.036 \times 10^{-3}T - 0.626 \times 10^{-5}T^{-2}$
 $H^\circ - H^\circ_{298} = 8.873 \times 10^{-3}T + 0.018 \times 10^{-6}T^2 + 0.626 \times 10^{-2}T^{-1} - 2.857$

Reaction equations (kcal/mol):

298.15-999 K: $\Delta H_r^\circ = 16.192 - 0.384 \times 10^{-3}T - 2.089 \times 10^{-6}T^2 + 45.650T^{-1}$
 $\Delta G_r^\circ = 16.192 + 0.384 \times 10^{-3}T \ln T + 2.089 \times 10^{-5}T^2 + 22.825T^{-1} - 21.134 \times 10^{-3}T$
999-1071 K: $\Delta H_r^\circ = 17.452 - 4.289 \times 10^{-3}T - 0.142 \times 10^{-6}T^2 + 28.450T^{-1}$
 $\Delta G_r^\circ = 17.452 + 4.289 \times 10^{-3}T \ln T + 0.142 \times 10^{-6}T^2 + 14.225T^{-1} - 47.413 \times 10^{-3}T$
1071-2000 K: $\Delta H_r^\circ = 16.169 - 4.309 \times 10^{-3}T - 0.142 \times 10^{-6}T^2 + 28.450T^{-1}$
 $\Delta G_r^\circ = 16.169 + 4.309 \times 10^{-3}T \ln T + 0.142 \times 10^{-6}T^2 + 14.225T^{-1} - 46.354 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (104). Other data are those estimated by Mills (80).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHf°	ΔGf°	
298.15	30.770	43.100	43.100	0	-284.000	-279.742	205.053
300*	30.790	43.290	43.100	.057	-283.997	-279.714	203.769
368.3	31.350	49.671	43.743	2.183	-283.917	-278.747	165.407
368.3	31.350	49.671	43.743	2.183	-284.205	-278.747	165.407
388.36	31.515	51.338	44.093	2.814	-284.200	-278.448	156.695
388.36	31.515	51.338	44.093	2.814	-285.439	-278.448	156.695
400	31.610	52.270	44.318	3.181	-285.493	-278.238	152.020
432.02	31.777	54.711	44.999	4.196	-285.704	-277.651	140.456
500	32.130	59.390	46.650	6.370	-286.501	-276.321	120.778
600	32.530	65.280	49.273	9.604	-287.292	-274.196	99.875
700	32.870	70.320	51.929	12.874	-287.950	-271.970	84.912
717.824	32.927	71.147	52.395	13.460	-288.055	-271.561	82.679

*Data above 298 K estimated.

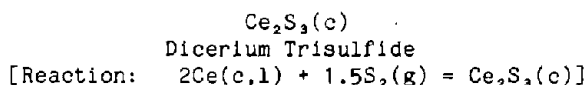
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta\text{H}^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta\text{H}^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta\text{H}^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $\text{Cp}^\circ = 31.321 + 2.560 \times 10^{-3}\text{T} - 1.168 \times 10^{-5}\text{T}^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 31.321 \times 10^{-3}\text{T} + 1.280 \times 10^{-6}\text{T}^2 + 1.168 \times 10^{-2}\text{T}^{-1} - 9.844$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta\text{Hf}^\circ = -282.162 - 3.371 \times 10^{-3}\text{T} + 2.537 \times 10^{-6}\text{T}^2 - 315.600\text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -282.162 + 3.371 \times 10^{-3}\text{T} \ln \text{T} - 2.537 \times 10^{-6}\text{T}^2 - 157.800\text{T}^{-1} - 8.557 \times 10^{-3}\text{T}$
 368.3-388.36 K: $\Delta\text{Hf}^\circ = -285.507 + 3.418 \times 10^{-3}\text{T} - 2.701 \times 10^{-6}\text{T}^2 + 151.200\text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -285.507 - 3.418 \times 10^{-3}\text{T} \ln \text{T} + 2.701 \times 10^{-6}\text{T}^2 + 75.600\text{T}^{-1} + 36.992 \times 10^{-3}\text{T}$
 388.36-432.02 K: $\Delta\text{Hf}^\circ = -333.982 + 137.638 \times 10^{-3}\text{T} - 132.547 \times 10^{-6}\text{T}^2 + 5857.800\text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -333.982 - 137.638 \times 10^{-3}\text{T} \ln \text{T} + 132.547 \times 10^{-6}\text{T}^2 + 2928.900\text{T}^{-1} + 892.677 \times 10^{-3}\text{T}$
 432.02-717.824 K: $\Delta\text{Hf}^\circ = -362.418 + 125.920 \times 10^{-3}\text{T} - 73.111 \times 10^{-6}\text{T}^2 + 15537.300\text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -362.418 - 125.920 \times 10^{-3}\text{T} \ln \text{T} + 73.111 \times 10^{-6}\text{T}^2 + 7768.650\text{T}^{-1} + 887.135 \times 10^{-3}\text{T}$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	30.770	43.100	43.100	0	-330.065	-308.282	225.974
300*	30.790	43.290	43.100	.057	-330.053	-308.146	224.481
400	31.610	52.270	44.318	3.181	-329.446	-300.935	164.421
500	32.130	59.390	46.650	6.370	-328.884	-293.880	128.453
600	32.530	65.280	49.273	9.604	-328.375	-286.919	104.509
700	32.870	70.320	51.929	12.874	-327.925	-280.056	87.436
800	33.190	74.730	54.508	16.178	-327.534	-273.229	74.642
900	33.480	78.660	56.981	19.511	-327.207	-266.472	64.707
999	33.757	82.166	59.304	22.839	-326.941	-259.808	56.837
999	33.757	82.166	59.304	22.839	-328.371	-259.808	56.837
1000	33.760	82.200	59.327	22.873	-328.369	-259.744	56.766
1071	33.959	84.522	60.919	25.278	-328.192	-254.866	52.007
1071	33.959	84.522	60.919	25.278	-330.802	-254.866	52.007
1100	34.040	85.430	61.554	26.264	-330.728	-252.810	50.228
1200	34.310	88.400	63.666	29.681	-330.467	-245.744	44.755
1300	34.580	91.160	65.678	33.126	-330.187	-238.702	40.129
1400	34.840	93.730	67.589	36.597	-329.893	-231.665	36.164
1500	35.110	96.150	69.420	40.095	-329.583	-224.676	32.735
1600	35.370	98.420	71.158	43.619	-329.258	-217.690	29.735
1700	35.630	100.570	72.824	47.169	-328.919	-210.712	27.088
1800	35.890	102.620	74.428	50.746	-328.560	-203.795	24.744
1900	36.150	104.570	75.966	54.348	-328.186	-196.868	22.645
2000	36.410	106.430	77.442	57.976	-327.796	-189.973	20.759

*Data above 298 K estimated.

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.

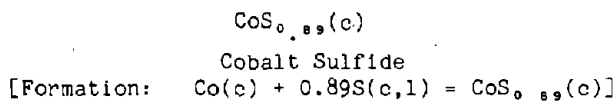
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 31.321 + 2.560 \times 10^{-3}T - 1.168 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 31.321 \times 10^{-3}T + 1.280 \times 10^{-6}T^2 + 1.168 \times 10^{-2}T^{-1} - 9.844$

Reaction equations (kcal/mol):

298.15-999 K: $\Delta H_r^\circ = -332.528 + 8.636 \times 10^{-3}T - 3.094 \times 10^{-6}T^2 + 48.750T^{-1}$
 $\Delta G_r^\circ = -332.528 - 8.636 \times 10^{-3}T \ln T + 3.094 \times 10^{-6}T^2 + 24.375T^{-1} + 129.332 \times 10^{-3}T$
999-1071 K: $\Delta H_r^\circ = -330.008 + 0.826 \times 10^{-3}T + 0.800 \times 10^{-6}T^2 + 14.350T^{-1}$
 $\Delta G_r^\circ = -330.008 - 0.826 \times 10^{-3}T \ln T - 0.800 \times 10^{-6}T^2 + 7.175T^{-1} + 76.775 \times 10^{-3}T$
1071-2000 K: $\Delta H_r^\circ = -332.575 + 0.786 \times 10^{-3}T + 0.800 \times 10^{-6}T^2 + 14.350T^{-1}$
 $\Delta G_r^\circ = -332.575 - 0.786 \times 10^{-3}T \ln T - 0.800 \times 10^{-6}T^2 + 7.175T^{-1} + 78.893 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (104). Low-temperature heat capacities and entropy at 298 K from King (66). Data above 298 K estimated.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	10.364	10.908	10.908	0	-50.630	-49.709	36.437
300*	10.390	10.972	10.909	.019	-50.631	-49.702	36.207
368.3	11.134	13.184	11.130	.757	-50.650	-49.494	29.369
368.3	11.134	13.184	11.130	.757	-50.735	-49.494	29.369
388.36	11.353	13.781	11.252	.982	-50.741	-49.425	27.814
388.36	11.353	13.781	11.252	.982	-51.109	-49.425	27.814
400	11.480	14.118	11.331	1.115	-51.128	-49.375	26.977
432.02	11.752	15.013	11.571	1.487	-51.195	-49.232	24.905
500	12.330	16.774	12.160	2.307	-51.425	-48.897	21.373
600	13.090	19.091	13.126	3.579	-51.608	-48.373	17.620
700	13.800	21.164	14.128	4.925	-51.702	-47.828	14.932
700	13.800	21.164	14.128	4.925	-51.810	-47.828	14.932
717.824	13.923	21.512	14.307	5.172	-51.815	-47.727	14.531

*Data above 298 K estimated.

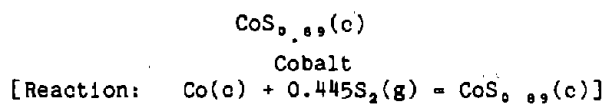
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
700 K, α - β transition point of Co; ΔH° = 0.108 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1000 K: Cp° = 9.452 + 6.478x10⁻³T - 0.906x10⁻⁵T²
H° - H₂₉₈° = 9.452x10⁻³T + 3.239x10⁻⁶T² + 0.906x10⁻²T⁻¹ - 3.410

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -49.854 - 2.824x10⁻³T + 2.990x10⁻⁶T² - 59.484T⁻¹
ΔGf° = -49.854 + 2.824x10⁻³T ln T - 2.990x10⁻⁶T² - 29.742T⁻¹ - 14.374x10⁻³T
368.3-388.36 K: ΔHf° = -50.847 - 0.810x10⁻³T + 1.436x10⁻⁶T² + 79.000T⁻¹
ΔGf° = -50.847 + 0.810x10⁻³T ln T - 1.436x10⁻⁶T² + 39.500T⁻¹ - 0.862x10⁻³T
388.36-432.02 K: ΔHf° = -65.228 + 39.009x10⁻³T - 37.085x10⁻⁶T² + 1771.958T⁻¹
ΔGf° = -65.228 - 39.009x10⁻³T ln T + 37.085x10⁻⁶T² + 885.979T⁻¹ + 252.992x10⁻³T
432.02-700 K: ΔHf° = -73.664 + 35.532x10⁻³T - 19.452x10⁻⁶T² + 4643.543T⁻¹
ΔGf° = -73.664 - 35.532x10⁻³T ln T + 19.452x10⁻⁶T² + 2321.771T⁻¹ + 251.348x10⁻³T
700-717.824 K: ΔHf° = -80.196 + 44.018x10⁻³T - 23.090x10⁻⁶T² + 6229.943T⁻¹
ΔGf° = -80.196 - 44.018x10⁻³T ln T + 23.090x10⁻⁶T² + 3114.972T⁻¹ + 312.106x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	10.364	10.908	10.908	0	-64.296	-58.176	42.643
300*	10.390	10.972	10.909	.019	-64.294	-58.137	42.352
400	11.480	14.118	11.331	1.115	-64.167	-56.108	30.656
500	12.330	16.774	12.160	2.307	-63.998	-54.107	23.650
600	13.090	19.091	13.126	3.579	-63.796	-52.147	18.994
700	13.800	21.164	14.128	4.925	-63.561	-50.227	15.681
700	13.800	21.164	14.128	4.925	-63.669	-50.227	15.681
800	14.490	23.052	15.128	6.339	-63.394	-48.321	13.201
900	15.150	24.797	16.107	7.821	-63.104	-46.457	11.281
1000	15.800	26.427	17.058	9.369	-62.805	-44.632	9.754

*Data above 298 K estimated.

Phase change: 700 K, α - β transition point of Co; ΔH° = 0.108 kcal/mol.

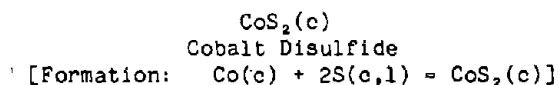
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $C_p^\circ = 9.452 + 6.478 \times 10^{-3}T - 0.906 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 9.452 \times 10^{-3}T + 3.239 \times 10^{-6}T^2 + 0.906 \times 10^{-2}T^{-1} - 3.410$

Reaction equations (kcal/mol):

298.15-700 K: $\Delta H_r^\circ = -64.796 + 0.738 \times 10^{-3}T + 1.320 \times 10^{-6}T^2 + 48.606T^{-1}$
 $\Delta G_r^\circ = -64.796 - 0.738 \times 10^{-3}T \ln T - 1.320 \times 10^{-6}T^2 + 24.303T^{-1} + 26.533 \times 10^{-3}T$
700-1000 K: $\Delta H_r^\circ = -71.328 + 9.224 \times 10^{-3}T - 2.318 \times 10^{-6}T^2 + 1635.006T^{-1}$
 $\Delta G_r^\circ = -71.328 - 9.224 \times 10^{-3}T \ln T + 2.318 \times 10^{-6}T^2 + 817.503T^{-1} + 87.291 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K, low-temperature heat capacities, and entropy at 298 K from Stuve (113). Data above 298 K estimated.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	16.313	17.876	17.876	0	-36.600	-35.221	25.817
300*	16.340	17.977	17.877	.030	-36.601	-35.211	25.651
368.3	17.303	21.436	18.223	1.183	-36.631	-34.897	20.708
368.3	17.303	21.436	18.223	1.183	-36.823	-34.897	20.708
388.36	17.586	22.361	18.413	1.533	-36.836	-34.790	19.578
388.36	17.586	22.361	18.413	1.533	-37.662	-34.790	19.578
400	17.750	22.883	18.535	1.739	-37.706	-34.704	18.961
432.02	18.086	24.263	18.910	2.313	-37.863	-34.459	17.432
500	18.800	26.961	19.825	3.568	-38.406	-33.869	14.804
600	19.700	30.470	21.313	5.494	-38.886	-32.914	11.989
700	20.520	33.568	22.847	7.505	-39.203	-31.894	9.958
700	20.520	33.568	22.847	7.505	-39.311	-31.894	9.958
717.824	20.659	34.086	23.119	7.872	-39.349	-31.705	9.653

*Data above 298 K estimated.

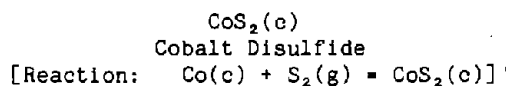
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 700 K, α - β transition point of Co; ΔH° = 0.108 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1000 K: Cp° = 15.731 + 7.248x10⁻³T - 1.403x10⁻⁵T²
 H° - H₂₉₈° = 15.731x10⁻³T + 3.624x10⁻⁶T² + 1.403x10⁻²T³ - 5.483

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -34.782 - 5.618x10⁻³T + 5.281x10⁻⁶T² - 182.500T⁻¹
 ΔGf° = -34.782 + 5.618x10⁻³T ln T - 5.281x10⁻⁶T² - 91.250T⁻¹ - 30.879x10⁻³T
 368.3-388.36 K: ΔHf° = -37.013 - 1.092x10⁻³T + 1.789x10⁻⁶T² + 128.700T⁻¹
 ΔGf° = -37.013 + 1.092x10⁻³T ln T - 1.789x10⁻⁶T² + 64.350T⁻¹ - 0.513x10⁻³T
 388.36-432.02 K: ΔHf° = -69.329 + 88.388x10⁻³T - 84.775x10⁻⁶T² + 3933.100T⁻¹
 ΔGf° = -69.329 - 88.388x10⁻³T ln T + 84.775x10⁻⁶T² + 1966.550T⁻¹ + 569.944x10⁻³T
 432.02-700 K: ΔHf° = -88.287 + 80.576x10⁻³T - 45.151x10⁻⁶T² + 10386.100T⁻¹
 ΔGf° = -88.287 - 80.576x10⁻³T ln T + 45.151x10⁻⁶T² + 5193.050T⁻¹ + 566.249x10⁻³T
 700-717.824 K: ΔHf° = -94.818 + 89.062x10⁻³T - 48.789x10⁻⁶T² + 11972.500T⁻¹
 ΔGf° = -94.818 - 89.062x10⁻³T ln T + 48.789x10⁻⁶T² + 5986.250T⁻¹ + 627.007x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	16.313	17.876	17.876	0	-67.310	-54.248	39.764
300*	16.340	17.977	17.877	.030	-67.305	-54.166	39.459
400	17.750	22.883	18.535	1.739	-67.008	-49.835	27.228
500	18.800	26.961	19.825	3.568	-66.661	-45.576	19.921
600	19.700	30.470	21.313	5.494	-66.275	-41.395	15.078
700	20.520	33.568	22.847	7.505	-65.853	-37.284	11.640
700	20.520	33.568	22.847	7.505	-65.961	-37.284	11.640
800	21.300	36.360	24.364	9.597	-65.492	-33.214	9.074
900	22.080	38.914	25.841	11.766	-65.003	-29.212	7.094
1000	22.850	41.280	27.268	14.012	-64.498	-25.271	5.523

*Data above 298 K estimated.

Phase change: 700 K, α - β transition point of Co; ΔH° = 0.108 kcal/mol.

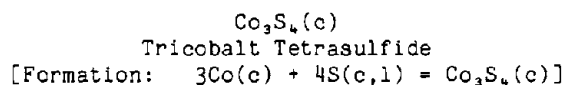
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $C_p^\circ = 15.731 + 7.248 \times 10^{-3}T - 1.403 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 15.731 \times 10^{-3}T + 3.624 \times 10^{-6}T^2 + 1.403 \times 10^{-2}T^{-1} - 5.483$

Reaction equations (kcal/mol):

298.15-700 K: $\Delta H_r^\circ = -68.360 + 2.387 \times 10^{-3}T + 1.527 \times 10^{-6}T^2 + 60.400T^{-1}$
 $\Delta G_r^\circ = -68.360 - 2.387 \times 10^{-3}T \ln T - 1.527 \times 10^{-6}T^2 + 30.200T^{-1} + 61.047 \times 10^{-3}T$
700-1000 K: $\Delta H_r^\circ = -74.892 + 10.873 \times 10^{-3}T - 2.111 \times 10^{-6}T^2 + 1646.800T^{-1}$
 $\Delta G_r^\circ = -74.892 - 10.873 \times 10^{-3}T \ln T + 2.111 \times 10^{-6}T^2 + 823.400T^{-1} + 121.806 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mills (80). Low-temperature heat capacities and entropy at 298 K from Stuve (113). Data above 298 K estimated.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHf°	ΔGf°	
298.15	38.870	42.050	42.050	0	-85.800	-82.779	60.678
300*	38.950	42.290	42.057	.070	-85.803	-82.758	60.288
368.3	41.340	50.551	42.889	2.822	-85.832	-82.080	48.706
368.3	41.340	50.551	42.889	2.822	-86.216	-82.080	48.706
388.36	42.043	52.762	43.343	3.658	-86.232	-81.851	46.061
388.36	42.043	52.762	43.343	3.658	-87.884	-81.851	46.061
400	42.450	54.010	43.635	4.150	-87.965	-81.671	44.622
432.02	43.337	57.313	44.528	5.523	-88.259	-81.158	41.056
500	45.220	63.790	46.710	8.540	-89.288	-79.929	34.936
600	47.610	72.240	50.273	13.180	-90.152	-77.967	28.399
700	49.790	79.750	53.964	18.050	-90.666	-75.905	23.698
700	49.790	79.750	53.964	18.050	-90.990	-75.905	23.698
717.824	50.155	81.006	54.620	18.941	-91.040	-75.523	22.994

*Data above 298 K estimated.

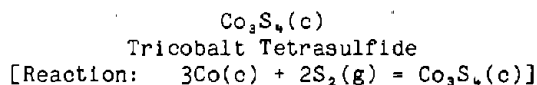
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta\text{H}^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta\text{H}^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta\text{H}^\circ = 0$ kcal/mol.
 700 K, $\alpha - \beta$ transition point of Co; $\Delta\text{H}^\circ = 0.108$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-900 K: $\text{Cp}^\circ = 36.601 + 19.724 \times 10^{-3}T - 3.211 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 36.601 \times 10^{-3}T + 9.862 \times 10^{-6}T^2 + 3.211 \times 10^{-2}T^{-1} - 12.866$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta\text{Hf}^\circ = -82.377 - 11.098 \times 10^{-3}T + 11.399 \times 10^{-6}T^2 - 336.100T^{-1}$
 $\Delta\text{Gf}^\circ = -82.377 + 11.098 \times 10^{-3}T \ln T - 11.399 \times 10^{-6}T^2 - 168.050T^{-1} - 59.289 \times 10^{-3}T$
 368.3-388.36 K: $\Delta\text{Hf}^\circ = -86.838 - 2.046 \times 10^{-3}T + 4.415 \times 10^{-6}T^2 + 286.300T^{-1}$
 $\Delta\text{Gf}^\circ = -86.838 + 2.046 \times 10^{-3}T \ln T - 4.415 \times 10^{-6}T^2 + 143.150T^{-1} + 1.443 \times 10^{-3}T$
 388.36-432.02 K: $\Delta\text{Hf}^\circ = -151.471 + 176.914 \times 10^{-3}T - 168.713 \times 10^{-6}T^2 + 7895.100T^{-1}$
 $\Delta\text{Gf}^\circ = -151.471 - 176.914 \times 10^{-3}T \ln T + 168.713 \times 10^{-6}T^2 + 3947.550T^{-1} + 1142.356 \times 10^{-3}T$
 432.02-700 K: $\Delta\text{Hf}^\circ = -189.386 + 161.290 \times 10^{-3}T - 89.465 \times 10^{-6}T^2 + 20801.100T^{-1}$
 $\Delta\text{Gf}^\circ = -189.386 - 161.290 \times 10^{-3}T \ln T + 89.465 \times 10^{-6}T^2 + 10400.550T^{-1} + 1134.966 \times 10^{-3}T$
 700-717.824 K: $\Delta\text{Hf}^\circ = -208.981 + 186.748 \times 10^{-3}T - 100.379 \times 10^{-6}T^2 + 25560.300T^{-1}$
 $\Delta\text{Gf}^\circ = -208.981 - 186.748 \times 10^{-3}T \ln T + 100.379 \times 10^{-6}T^2 + 12780.150T^{-1} + 1317.241 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHr°	ΔGr°	
298.15	38.870	42.050	42.050	0	-147.220	-120.833	88.572
300*	38.950	42.290	42.057	.070	-147.211	-120.667	87.905
400	42.450	54.010	43.635	4.150	-146.569	-111.933	61.157
500	45.220	63.790	46.710	8.540	-145.798	-103.342	45.170
600	47.610	72.240	50.273	13.180	-144.930	-94.931	34.578
700	49.790	79.750	53.964	18.050	-143.966	-86.686	27.064
700	49.790	79.750	53.964	18.050	-144.290	-86.686	27.064
800	51.840	86.530	57.605	23.140	-143.198	-78.507	21.447
900	53.800	92.750	61.172	28.420	-142.078	-70.497	17.119

*Data above 298 K estimated.

Phase change: 700 K, $\alpha - \beta$ transition point of Co; $\Delta\text{H}^\circ = 0.108$ kcal/mol.

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

298.15-900 K: $\text{Cp}^\circ = 36.601 + 19.724 \times 10^{-3}T - 3.211 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 36.601 \times 10^{-3}T + 9.862 \times 10^{-6}T^2 + 3.211 \times 10^{-2}T^{-1} - 12.866$

Reaction equations (kcal/mol):

298.15-700 K: $\Delta\text{Hr}^\circ = -149.532 + 4.912 \times 10^{-3}T + 3.891 \times 10^{-6}T^2 + 149.700T^{-1}$
 $\Delta\text{Gr}^\circ = -149.532 - 4.912 \times 10^{-3}T \ln T - 3.891 \times 10^{-6}T^2 + 74.850T^{-1} + 124.563 \times 10^{-3}T$
 700-900 K: $\Delta\text{Hr}^\circ = -169.128 + 30.370 \times 10^{-3}T - 7.023 \times 10^{-6}T^2 + 4908.900T^{-1}$
 $\Delta\text{Gr}^\circ = -169.128 - 30.370 \times 10^{-3}T \ln T + 7.023 \times 10^{-6}T^2 + 2454.450T^{-1} + 306.838 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mills (80). Low-temperature heat capacities and entropy at 298 K from Stuve (113). Data above 298 K estimated.

CrS(c)
Chromium Monosulfide
[Formation: Cr(c) + S(c,1) = CrS(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(C° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15*	11.160	15.300	15.300	0	-32.300	-32.893	24.111
300	11.180	15.370	15.300	.021	-32.299	-32.897	23.966
311.5	11.302	15.793	15.310	.150	-32.300	-32.920	23.097
368.3	11.904	17.583	15.532	.755	-32.330	-33.032	19.601
368.3	11.904	17.583	15.532	.755	-32.426	-33.032	19.601
388.36	12.117	18.220	15.655	.996	-32.432	-33.065	18.607
388.36	12.117	18.220	15.655	.996	-32.845	-33.065	18.607
400	12.240	18.580	15.735	1.138	-32.863	-33.071	18.069
432.02	13.617	19.570	15.982	1.550	-32.908	-33.086	16.737
450	14.480	20.140	16.133	1.803	-32.990	-33.089	16.070
500	12.930	21.540	16.604	2.468	-33.092	-33.093	14.465
600	13.050	23.910	17.632	3.767	-33.308	-33.073	12.047
700	13.160	25.930	18.677	5.077	-33.485	-33.019	10.309
717.824	13.181	26.261	18.861	5.312	-33.512	-33.006	10.049

*Entropy at 298 K estimated and data extrapolated above 670 K.

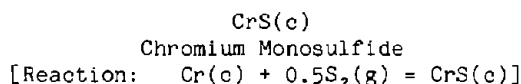
Phase changes: 311.5 K, second order transition point of Cr; ΔH° = 0 kcal/mol.
368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
450 K, second order transition point of CrS; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-450 K: Cp° = -29.882 + 82.496x10⁻³T + 14.620x10⁵T⁻²
H° - H₂₉₈° = -29.882x10⁻³T + 41.248x10⁻⁶T² - 14.620x10²T⁻¹ + 10.146
450-1800 K: Cp° = 9.210 + 3.154x10⁻³T + 7.798x10⁵T⁻²
H° - H₂₉₈° = 9.210x10⁻³T + 1.577x10⁻⁶T² - 7.798x10²T⁻¹ - 0.928

Formation equations (kcal/mol):

298.15-311.5 K: ΔHf° = -18.934 - 35.248x10⁻³T + 28.898x10⁻⁶T² - 1617.600T⁻¹
ΔGf° = -18.934 + 35.248x10⁻³T lnT - 28.898x10⁻⁶T² - 808.800T⁻¹ - 229.933x10⁻³T
311.5-368.3 K: ΔHf° = -17.937 - 42.415x10⁻³T + 41.174x10⁻⁶T² - 1604.000T⁻¹
ΔGf° = -17.937 + 42.415x10⁻³T lnT - 41.174x10⁻⁶T² - 802.000T⁻¹ - 270.530x10⁻³T
368.3-388.36 K: ΔHf° = -19.052 - 40.152x10⁻³T + 39.428x10⁻⁶T² - 1448.400T⁻¹
ΔGf° = -19.052 + 40.152x10⁻³T lnT - 39.428x10⁻⁶T² - 724.200T⁻¹ - 255.347x10⁻³T
388.36-432.02 K: ΔHf° = -35.210 + 4.588x10⁻³T - 3.854x10⁻⁶T² + 453.800T⁻¹
ΔGf° = -35.210 - 4.588x10⁻³T lnT + 3.854x10⁻⁶T² + 226.900T⁻¹ + 29.881x10⁻³T
432.02-450 K: ΔHf° = -44.689 + 0.682x10⁻³T + 15.958x10⁻⁶T² + 3680.300T⁻¹
ΔGf° = -44.689 - 0.682x10⁻³T lnT - 15.958x10⁻⁶T² + 1840.150T⁻¹ + 28.034x10⁻³T
450-717.824 K: ΔHf° = -55.763 + 39.774x10⁻³T - 23.713x10⁻⁶T² + 4362.500T⁻¹
ΔGf° = -55.763 - 39.774x10⁻³T lnT + 23.713x10⁻⁶T² + 2181.250T⁻¹ + 271.929x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15*	11.160	15.300	15.300	0	-47.655	-42.407	31.085
300	11.180	15.370	15.300	.021	-47.651	-42.375	30.870
311.5	11.302	15.793	15.310	.150	-47.634	-42.173	29.588
400	12.240	18.580	15.735	1.138	-47.514	-40.637	22.203
450	14.480	20.140	16.133	1.803	-47.361	-39.782	19.320
500	12.930	21.540	16.604	2.468	-47.219	-38.947	17.023
600	13.050	23.910	17.632	3.767	-47.002	-37.314	13.591
700	13.160	25.930	18.677	5.077	-46.810	-35.714	11.150
800	13.280	27.700	19.700	6.400	-46.635	-34.144	9.328
900	13.400	29.270	20.677	7.734	-46.471	-32.592	7.914
1000	13.520	30.690	21.611	9.079	-46.321	-31.062	6.789
1100	13.630	31.980	22.492	10.437	-46.196	-29.537	5.868
1200	13.750	33.170	23.332	11.806	-46.103	-28.021	5.103
1300	13.870	34.280	24.138	13.185	-46.049	-26.535	4.461
1400	13.980	35.310	24.896	14.579	-46.022	-25.035	3.908
1500	14.100	36.280	25.625	15.983	-46.027	-23.527	3.428
1600	14.220	37.190	26.316	17.399	-46.068	-22.020	3.008
1700	14.340	38.060	26.985	18.827	-46.144	-20.534	2.640
1800	14.450	38.880	27.621	20.266	-46.250	-19.008	2.308

*Entropy at 298 K estimated and data extrapolated above 670 K.

Phase changes: 311.5 K, second order transition point of Cr; $\Delta H^\circ = 0$ kcal/mol.
450 K, second order transition point of CrS; $\Delta H^\circ = 0$ kcal/mol.

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

$$\begin{aligned}
 298.15-450 \text{ K: } & \text{Cp}^\circ = -29.882 + 82.496 \times 10^{-3}T + 14.620 \times 10^{-5}T^{-2} \\
 & \text{H}^\circ - \text{H}_{298}^\circ = -29.882 \times 10^{-3}T + 41.248 \times 10^{-6}T^2 - 14.620 \times 10^{-2}T^{-1} + 10.146 \\
 450-1800 \text{ K: } & \text{Cp}^\circ = 9.210 + 3.154 \times 10^{-3}T + 7.798 \times 10^{-5}T^{-2} \\
 & \text{H}^\circ - \text{H}_{298}^\circ = 9.210 \times 10^{-3}T + 1.577 \times 10^{-6}T^2 - 7.798 \times 10^{-2}T^{-1} - 0.928
 \end{aligned}$$

Reaction equations (kcal/mol):

$$\begin{aligned}
 298.15-311.5 \text{ K: } & \Delta \text{Hr}^\circ = -35.723 - 31.246 \times 10^{-3}T + 27.021 \times 10^{-6}T^2 - 1496.150T^{-1} \\
 & \Delta \text{Gr}^\circ = -35.723 + 31.246 \times 10^{-3}T \ln T - 27.021 \times 10^{-6}T^2 - 748.075T^{-1} - 183.970 \times 10^{-3}T \\
 311.5-450 \text{ K: } & \Delta \text{Hr}^\circ = -34.725 - 38.412 \times 10^{-3}T + 39.297 \times 10^{-6}T^2 - 1482.550T^{-1} \\
 & \Delta \text{Gr}^\circ = -34.725 + 38.412 \times 10^{-3}T \ln T - 39.297 \times 10^{-6}T^2 - 741.275T^{-1} - 224.567 \times 10^{-3}T \\
 450-1800 \text{ K: } & \Delta \text{Hr}^\circ = -45.799 + 0.679 \times 10^{-3}T - 0.374 \times 10^{-6}T^2 - 800.350T^{-1} \\
 & \Delta \text{Gr}^\circ = -45.799 - 0.679 \times 10^{-3}T \ln T + 0.374 \times 10^{-6}T^2 - 400.175T^{-1} + 19.328 \times 10^{-3}T
 \end{aligned}$$

Source: Data from Mills (80) who estimated entropy at 298 K and extrapolated data above 670 K.

$\text{Cr}_2\text{S}_3(\text{c})$
Dichromium Trisulfide
[Formation: $2\text{Cr}(\text{c}) + 3\text{S}(\text{c},1) = \text{Cr}_2\text{S}_3(\text{c})$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHf°	ΔGf°	
298.15*	26.810	35.600	35.600	0	-81.500	-81.893	60.028
300	26.810	35.770	35.603	.050	-81.500	-81.898	59.662
311.5	26.877	36.780	35.628	.359	-81.514	-81.912	57.469
368.3	27.206	41.296	36.152	1.895	-81.570	-81.974	48.643
368.3	27.206	41.296	36.152	1.895	-81.858	-81.974	48.643
388.36	27.322	42.742	36.455	2.442	-81.925	-81.977	46.132
388.36	27.322	42.742	36.455	2.442	-83.164	-81.977	46.132
400	27.390	43.550	36.650	2.760	-83.252	-81.941	44.770
432.02	27.669	45.670	37.241	3.641	-83.549	-81.827	41.394
500	28.260	49.750	38.670	5.540	-84.527	-81.467	35.609
600	29.240	54.990	40.973	8.410	-85.544	-80.758	29.416
700	30.280	59.570	43.299	11.390	-86.338	-79.885	24.941
717.824	30.471	60.334	43.712	11.931	-86.458	-79.718	24.271

*Entropy at 298 K estimated.

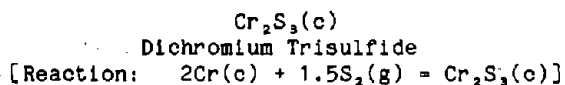
Phase changes: 311.5 K, second order transition point of Cr; $\Delta\text{H}^\circ = 0$ kcal/mol.
 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta\text{H}^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta\text{H}^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta\text{H}^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-1500 K: $\text{Cp}^\circ = 22.190 + 11.234 \times 10^{-3}\text{T} + 1.129 \times 10^{-5}\text{T}^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 22.190 \times 10^{-3}\text{T} + 5.617 \times 10^{-6}\text{T}^2 - 1.129 \times 10^{-2}\text{T}^{-1} - 6.737$

Formation equations (kcal/mol):

298.15-311.5 K: $\Delta\text{Hf}^\circ = -78.991 + 3.284 \times 10^{-3}\text{T} - 17.366 \times 10^{-6}\text{T}^2 - 579.700\text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -78.991 - 3.284 \times 10^{-3}\text{T} \ln \text{T} + 17.366 \times 10^{-6}\text{T}^2 - 289.850\text{T}^{-1} + 7.062 \times 10^{-3}\text{T}$
 311.5-368.3 K: $\Delta\text{Hf}^\circ = -76.996 - 11.050 \times 10^{-3}\text{T} + 7.186 \times 10^{-6}\text{T}^2 - 552.500\text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -76.996 + 11.050 \times 10^{-3}\text{T} \ln \text{T} - 7.186 \times 10^{-6}\text{T}^2 - 276.250\text{T}^{-1} - 74.133 \times 10^{-3}\text{T}$
 368.3-388.36 K: $\Delta\text{Hf}^\circ = -80.341 - 4.261 \times 10^{-3}\text{T} + 1.948 \times 10^{-6}\text{T}^2 - 85.700\text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -80.341 + 4.261 \times 10^{-3}\text{T} \ln \text{T} - 1.948 \times 10^{-6}\text{T}^2 - 42.850\text{T}^{-1} - 28.584 \times 10^{-3}\text{T}$
 388.36-432.02 K: $\Delta\text{Hf}^\circ = -128.816 + 129.959 \times 10^{-3}\text{T} - 127.898 \times 10^{-6}\text{T}^2 + 5620.900\text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -128.816 - 129.959 \times 10^{-3}\text{T} \ln \text{T} + 127.898 \times 10^{-6}\text{T}^2 + 2810.450\text{T}^{-1} + 827.101 \times 10^{-3}\text{T}$
 432.02-717.824 K: $\Delta\text{Hf}^\circ = -157.252 + 118.241 \times 10^{-3}\text{T} - 68.462 \times 10^{-6}\text{T}^2 + 15300.400\text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -157.252 - 118.241 \times 10^{-3}\text{T} \ln \text{T} + 68.462 \times 10^{-6}\text{T}^2 + 7650.200\text{T}^{-1} + 821.558 \times 10^{-3}\text{T}$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H° ₂₉₈)/T	H°- H° ₂₉₈	ΔHr°	ΔGr°	
298.15*	26.810	35.600	35.600	0	-127.565	-110.434	80.949
300	26.810	35.770	35.603	.050	-127.556	-110.329	80.374
311.5	26.877	36.780	35.628	.359	-127.516	-109.669	76.943
400	27.390	43.550	36.650	2.760	-127.205	-104.638	57.171
500	28.260	49.750	38.670	5.540	-126.910	-99.026	43.284
600	29.240	54.990	40.973	8.410	-126.628	-93.481	34.050
700	30.280	59.570	43.299	11.390	-126.313	-87.971	27.465
800	31.350	63.690	45.603	14.470	-125.964	-82.523	22.544
900	32.440	67.440	47.818	17.660	-125.553	-77.113	18.725
1000	33.540	70.920	49.960	20.960	-125.088	-71.762	15.683
1100	34.640	74.160	52.005	24.370	-124.593	-66.441	13.200
1200	35.750	77.230	53.988	27.890	-124.074	-61.179	11.142
1300	36.860	80.130	55.884	31.520	-123.549	-55.971	9.409
1400	37.980	82.900	57.714	35.260	-123.003	-50.800	7.930
1500	39.090	85.560	59.487	39.110	-122.431	-45.648	6.651

*Entropy at 298 K estimated.

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:

298.15-1500 K: $C_p^\circ = 22.190 + 11.234 \times 10^{-3}T + 1.129 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 22.190 \times 10^{-3}T + 5.617 \times 10^{-6}T^2 - 1.129 \times 10^{-2}T^{-1} - 6.737$

Reaction equations (kcal/mol):

298.15-311.5 K: $\Delta H_r^\circ = -129.358 + 15.292 \times 10^{-3}T - 22.997 \times 10^{-6}T^2 - 215.350T^{-1}$
 $\Delta G_r^\circ = -129.358 - 15.292 \times 10^{-3}T \ln T + 22.997 \times 10^{-6}T^2 - 107.675T^{-1} + 144.951 \times 10^{-3}T$
311.5-1500 K: $\Delta H_r^\circ = -127.362 + 0.957 \times 10^{-3}T + 1.555 \times 10^{-6}T^2 - 188.150T^{-1}$
 $\Delta G_r^\circ = -127.362 - 0.957 \times 10^{-3}T \ln T - 1.555 \times 10^{-6}T^2 - 94.075T^{-1} + 63.756 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Tret'yakov (120). Estimated entropy at 298 K from Mills (80). Other data based on relative enthalpy equation from Volovik (125).

CuFeS₂(c)
Copper Iron Sulfide, Chalcopyrite
[Formation: Cu(c) + Fe(c) + 2S(c,l) = CuFeS₂(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	22.888	29.873	29.873	0	-41.400	-41.432	30.370
300	22.937	30.015	29.875	.042	-41.400	-41.432	30.183
368.3	24.590	34.905	30.362	1.673	-41.362	-41.443	24.592
368.3	24.590	34.905	30.362	1.673	-41.554	-41.443	24.592
388.36	25.075	36.222	30.631	2.171	-41.543	-41.435	23.317
388.36	25.075	36.222	30.631	2.171	-42.369	-41.435	23.317
400	25.357	36.967	30.804	2.465	-42.397	-41.407	22.624
432.02	25.776	38.936	31.335	3.284	-42.511	-41.325	20.905
500	26.664	42.785	32.635	5.075	-42.955	-41.098	17.964
600	27.397	47.712	34.749	7.778	-43.329	-40.688	14.820
700	28.815	52.024	36.914	10.577	-43.564	-40.226	12.559
717.824	29.453	52.756	37.298	11.096	-43.583	-40.140	12.221

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-830 K: Cp° = 21.192 + 12.406x10⁻³T - 1.780x10⁻⁵T²
H° - H₂₉₈° = 21.192x10⁻³T + 6.203x10⁻⁶T² + 1.780x10⁻²T³ - 7.467

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -41.912 - 0.255x10⁻³T + 2.756x10⁻⁶T² + 102.300T⁻¹
ΔGf° = -41.912 + 0.255x10⁻³T ln T - 2.756x10⁻⁶T² + 51.150T⁻¹ + 0.404x10⁻³T
368.3-388.36 K: ΔHf° = -44.142 + 4.271x10⁻³T - 0.736x10⁻⁶T² + 413.500T⁻¹
ΔGf° = -44.142 - 4.271x10⁻³T ln T + 0.736x10⁻⁶T² + 206.750T⁻¹ + 30.770x10⁻³T
388.36-432.02 K: ΔHf° = -76.459 + 93.751x10⁻³T - 87.300x10⁻⁶T² + 4217.900T⁻¹
ΔGf° = -76.459 - 93.751x10⁻³T ln T + 87.300x10⁻⁶T² + 2108.950T⁻¹ + 601.227x10⁻³T
432.02-717.824 K: ΔHf° = -95.416 + 85.939x10⁻³T - 47.676x10⁻⁶T² + 10670.900T⁻¹
ΔGf° = -95.416 - 85.939x10⁻³T ln T + 47.676x10⁻⁶T² + 5335.450T⁻¹ + 597.532x10⁻³T

CuFeS₂(c,l)
Copper Iron Sulfide, Chalcopyrite
[Reaction: Cu(c,l) + Fe(c) + S₂(g) = CuFeS₂(c,l)]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(Cp° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	22.888	29.873	29.873	0	-72.110	-60.459	44.317
300	22.937	30.015	29.875	.042	-72.104	-60.387	43.991
400	25.357	36.967	30.804	2.465	-71.699	-56.539	30.891
500	26.664	42.785	32.635	5.075	-71.210	-52.804	23.081
600	27.397	47.712	34.749	7.778	-70.718	-49.170	17.910
700	28.815	52.024	36.914	10.577	-70.214	-45.617	14.242
800	32.398	56.073	39.057	13.613	-69.565	-42.144	11.513
830	34.128	57.295	39.693	14.610	-69.306	-41.120	10.827
830	36.743	60.187	39.693	17.010	-66.906	-41.120	10.827
900	46.231	63.166	41.400	19.589	-66.094	-38.976	9.465
930	74.960	65.094	42.132	21.355	-65.115	-38.086	8.950
930	41.200	65.094	42.132	21.355	-65.115	-38.086	8.950
1000	41.200	68.084	43.845	24.239	-64.143	-36.089	7.887
1043	41.200	69.819	44.880	26.011	-63.685	-34.893	7.311
1100	41.200	72.010	46.229	28.359	-62.942	-33.337	6.623
1155	41.200	74.020	47.505	30.625	-62.142	-31.876	6.032
1155	32.820	83.583	47.505	41.670	-51.097	-31.876	6.032
1185	32.820	84.425	48.430	42.655	-50.903	-31.380	5.787
1185	32.820	84.425	48.430	42.655	-51.118	-31.380	5.787
1200	32.820	84.838	48.882	43.147	-50.992	-31.132	5.670
1300	32.820	87.465	51.750	46.429	-50.185	-29.511	4.961
1357.6	32.820	88.888	53.296	48.319	-49.754	-28.606	4.605
1357.6	32.820	88.888	53.296	48.319	-52.874	-28.606	4.605
1400	32.820	89.897	54.389	49.711	-52.562	-27.853	4.348
1500	32.820	92.161	56.832	52.993	-51.845	-26.114	3.805

Phase changes: 830 K, transformation point of chalcopyrite to intermediate solid solution (ISS) + pyrite; ΔH° = 2.400 kcal/mol.

930 K, ISS + pyrite to ISS + pyrite + S(l); ΔH° = 0. kcal/mol.

1043 K, Curie temperature of Fe; ΔH° = 0 kcal/mol.

1155 K, ISS + pyrite + S(l) to liquid CuFeS₂; ΔH° = 11.045 kcal/mol.

1185 K, α - γ transition point of Fe; ΔH° = 0.215 kcal/mol.

1357.6 K, melting point of Cu; ΔH° = 3.120 kcal/mol.

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

298.15-830 K: Cp° = 21.192 + 12.406x10⁻³T - 1.780x10⁻⁵T²
H° - H₂₉₈° = 21.192x10⁻³T + 6.203x10⁻⁶T² + 1.780x10⁻²T³ - 7.467

830-930 K: Cp° = -344.170 + 440.476x10⁻³T
H° - H₂₉₈° = -344.170x10⁻³T + 220.238x10⁻⁶T² + 150.949

930-1155 K: Cp° = 41.200
H° - H₂₉₈° = 41.200x10⁻³T - 16.961

1155-1500 K: Cp° = 32.820
H° - H₂₉₈° = 32.820x10⁻³T + 3.763

Reaction equations (kcal/mol):

298.15-830 K: ΔHr° = -75.490 + 7.750x10⁻³T - 0.998x10⁻⁶T² + 345.200T⁻¹
ΔGr° = -75.490 - 7.750x10⁻³T lnT + 0.998x10⁻⁶T² + 172.600T⁻¹ + 92.330x10⁻³T

830-930 K: ΔHr° = 82.926 - 357.612x10⁻³T + 213.037x10⁻⁶T² + 167.200T⁻¹
ΔGr° = 82.926 + 357.612x10⁻³T lnT - 213.037x10⁻⁶T² + 83.600T⁻¹ - 2376.508x10⁻³T

930-1043 K: ΔHr° = -84.984 + 27.758x10⁻³T - 7.201x10⁻⁶T² + 167.200T⁻¹
ΔGr° = -84.984 - 27.758x10⁻³T lnT + 7.201x10⁻⁶T² + 83.600T⁻¹ + 233.294x10⁻³T

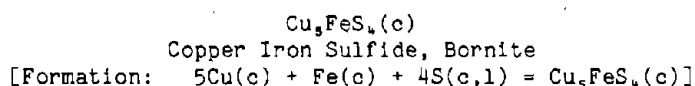
1043-1155 K: ΔHr° = -61.423 - 16.223x10⁻³T + 13.510x10⁻⁶T² - 61.300T⁻¹
ΔGr° = -61.423 + 16.223x10⁻³T lnT - 13.510x10⁻⁶T² - 30.650T⁻¹ - 73.250x10⁻³T

1155-1185 K: ΔHr° = -40.699 - 24.603x10⁻³T + 13.510x10⁻⁶T² - 61.300T⁻¹
ΔGr° = -40.699 + 24.603x10⁻³T lnT - 13.510x10⁻⁶T² - 30.650T⁻¹ - 150.287x10⁻³T

1185-1357.6 K: ΔHr° = -64.313 + 13.652x10⁻³T - 2.181x10⁻⁶T² + 57.700T⁻¹
ΔGr° = -64.313 - 13.652x10⁻³T lnT + 2.181x10⁻⁶T² + 28.850T⁻¹ + 121.753x10⁻³T

1357.6-1500 K: ΔHr° = -65.554 + 11.172x10⁻³T - 1.371x10⁻⁶T² + 50.700T⁻¹
ΔGr° = -65.554 - 11.172x10⁻³T lnT + 1.371x10⁻⁶T² + 25.350T⁻¹ + 105.880x10⁻³T

Sources: Enthalpy of formation at 298 K from Johnson (58). Low-temperature heat capacities and entropy at 298 K from King (64). High-temperature data based on Pankratz (94) and Conard (24).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	58.706	86.600	86.600	0	-90.900	-93.827	68.776
300	58.786	86.963	86.603	.108	-90.898	-93.844	68.365
368.3	61.627	99.309	87.842	4.224	-90.759	-94.529	56.093
368.3	61.627	99.309	87.842	4.224	-91.143	-94.529	56.093
388.36	62.462	102.600	88.520	5.468	-91.104	-94.712	53.299
388.36	62.462	102.600	88.520	5.468	-92.756	-94.712	53.299
400	62.946	104.452	88.957	6.198	-92.804	-94.771	51.780
432.02	64.192	109.347	90.289	8.233	-93.002	-94.923	48.019
485	66.254	116.892	92.789	11.690	-93.663	-95.110	42.858
485	85.082	119.840	92.789	13.120	-92.233	-95.110	42.858
500	89.024	122.491	93.641	14.425	-92.067	-95.202	41.612
540	99.534	129.742	96.048	18.195	-91.253	-95.483	38.644
600	79.308	138.160	99.850	22.986	-90.801	-95.977	34.959
700	77.983	150.275	106.214	30.843	-90.134	-96.892	30.251
717.824	77.900	152.234	107.332	32.232	-90.017	-97.064	29.552

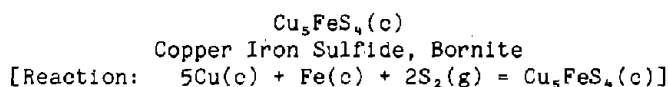
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
485 K, transition point of Cu₅FeS₄; ΔH° = 1.430 kcal/mol.
540 K, transition point of Cu₅FeS₄; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-485 K: Cp° = 48.668 + 37.088x10⁻³T - 0.906x10⁻⁵T²
H° - H₂₉₈° = 48.668x10⁻³T + 18.544x10⁻⁶T² + 0.906x10⁻²T⁻¹ - 16.463
485-540 K: Cp° = -34.310 + 247.000x10⁻³T
H° - H₂₉₈° = -34.310x10⁻³T + 123.500x10⁻⁶T² + 0.710
540-1200 K: Cp° = 80.330 - 2.040x10⁻³T
H° - H₂₉₈° = 80.330x10⁻³T - 1.020x10⁻⁶T² - 24.886

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -88.257 - 10.407x10⁻³T + 15.291x10⁻⁶T² - 268.300T⁻¹
ΔGf° = -88.257 + 10.407x10⁻³TlnT - 15.291x10⁻⁶T² - 134.150T⁻¹ - 71.909x10⁻³T
368.3-388.36 K: ΔHf° = -92.717 - 1.355x10⁻³T + 8.307x10⁻⁶T² + 354.100T⁻¹
ΔGf° = -92.717 + 1.355x10⁻³TlnT - 8.307x10⁻⁶T² + 177.050T⁻¹ - 11.177x10⁻³T
388.36-432.02 K: ΔHf° = -157.350 + 177.605x10⁻³T - 164.821x10⁻⁶T² + 7962.900T⁻¹
ΔGf° = -157.350 - 177.605x10⁻³TlnT + 164.821x10⁻⁶T² + 3981.450T⁻¹ + 1129.736x10⁻³T
432.02-485 K: ΔHf° = -195.265 + 161.981x10⁻³T - 85.573x10⁻⁶T² + 20868.900T⁻¹
ΔGf° = -195.265 - 161.981x10⁻³TlnT + 85.573x10⁻⁶T² + 10434.450T⁻¹ + 1122.346x10⁻³T
485-540 K: ΔHf° = -178.092 + 79.003x10⁻³T + 19.383x10⁻⁶T² + 20778.300T⁻¹
ΔGf° = -178.092 - 79.003x10⁻³TlnT - 19.383x10⁻⁶T² + 10389.150T⁻¹ + 624.886x10⁻³T
540-717.824 K: ΔHf° = -203.688 + 193.643x10⁻³T - 105.137x10⁻⁶T² + 20778.300T⁻¹
ΔGf° = -203.688 - 193.643x10⁻³TlnT + 105.137x10⁻⁶T² + 10389.150T⁻¹ + 1326.310x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	58.706	86.600	86.600	0	-152.320	-131.881	96.670
300	58.786	86.963	86.603	.108	-152.306	-131.753	95.981
400	62.946	104.452	88.957	6.198	-151.408	-125.033	68.314
485	66.254	116.892	92.789	11.690	-150.492	-119.521	53.858
485	85.082	119.840	92.789	13.120	-149.062	-119.521	53.858
500	89.024	122.491	93.641	14.425	-148.577	-118.615	51.846
540	99.534	129.742	96.048	18.195	-147.013	-116.278	47.059
600	79.308	138.160	99.850	22.986	-145.579	-112.940	41.138
700	77.983	150.275	106.214	30.843	-143.434	-107.673	33.617
800	77.518	160.648	112.384	38.611	-141.528	-102.696	28.055
900	77.914	169.793	118.264	46.376	-139.800	-97.948	23.785
1000	79.172	178.059	123.836	54.223	-138.243	-93.383	20.409
1043	80.083	181.411	126.141	57.647	-137.698	-91.466	19.166
1100	81.290	185.698	129.117	62.239	-136.809	-88.959	17.674
1185	83.822	191.835	133.397	69.248	-135.247	-85.319	15.735
1185	83.822	191.835	133.397	69.248	-135.462	-85.319	15.735
1200	84.269	192.892	134.135	70.509	-135.139	-84.687	15.423

Phase changes: 485 K, transition point of Cu₅FeS₄; ΔH° = 1.430 kcal/mol.
540 K, transition point of Cu₅FeS₄; ΔH° = 0 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.

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

298.15-485 K: Cp° = 48.668 + 37.088x10⁻³T - 0.906x10⁻⁵T²
H° - H₂₉₈° = 48.668x10⁻³T + 18.544x10⁻⁶T² + 0.906x10⁻²T³ - 16.463
485-540 K: Cp° = -34.310 + 247.000x10⁻³T
H° - H₂₉₈° = -34.310x10⁻³T + 123.500x10⁻⁶T² + 0.710
540-1200 K: Cp° = 80.330 - 2.040x10⁻³T
H° - H₂₉₈° = 80.330x10⁻³T - 1.020x10⁻⁶T² - 24.886

Reaction equations (kcal/mol):

298.15-485 K: ΔHr° = -155.412 + 5.603x10⁻³T + 7.783x10⁻⁶T² + 217.500T⁻¹
ΔGr° = -155.412 - 5.603x10⁻³T lnT - 7.783x10⁻⁶T² + 108.750T⁻¹ + 111.943x10⁻³T
485-540 K: ΔHr° = -138.239 - 77.375x10⁻³T + 112.739x10⁻⁶T² + 126.900T⁻¹
ΔGr° = -138.239 + 77.375x10⁻³T lnT - 112.739x10⁻⁶T² + 63.450T⁻¹ - 385.517x10⁻³T
540-1043 K: ΔHr° = -163.835 + 37.265x10⁻³T - 11.781x10⁻⁶T² + 126.900T⁻¹
ΔGr° = -163.835 - 37.265x10⁻³T lnT + 11.781x10⁻⁶T² + 63.450T⁻¹ + 315.907x10⁻³T
1043-1185 K: ΔHr° = -140.274 - 6.716x10⁻³T + 8.930x10⁻⁶T² - 101.600T⁻¹
ΔGr° = -140.274 + 6.716x10⁻³T lnT - 8.930x10⁻⁶T² - 50.800T⁻¹ + 9.362x10⁻³T
1185-1200 K: ΔHr° = -163.888 + 31.539x10⁻³T - 6.761x10⁻⁶T² + 17.400T⁻¹
ΔGr° = -163.888 - 31.539x10⁻³T lnT + 6.761x10⁻⁶T² + 8.700T⁻¹ + 281.403x10⁻³T

Source: Data from King (64).

$\text{Cu}_6\text{PS}_3\text{Br(c)}$
Copper Bromide Phosphorotetrathioate Sulfide
[Formation: $6\text{Cu(c)} + \text{P(c,l)} + 5\text{S(c,l)} + 0.5\text{Br}_2(\text{l,g}) = \text{Cu}_6\text{PS}_3\text{Br(c)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHf°	ΔGf°	
298.15	74.170	118.400	118.400	0	-114.000	-115.354	84.556
300	74.200	118.860	118.400	.140	-114.004	-115.359	84.038
317.3	74.466	123.028	118.533	1.426	-114.055	-115.435	79.508
317.3	74.466	123.028	118.533	1.426	-114.212	-115.435	79.508
332.6	74.702	126.534	118.843	2.558	-114.281	-115.499	75.893
332.6	74.702	126.534	118.843	2.558	-117.814	-115.499	75.893
350	74.970	130.350	119.321	3.860	-117.810	-115.380	72.046
368.3	75.263	134.178	119.965	5.235	-117.810	-115.254	68.391
368.3	75.263	134.178	119.965	5.235	-118.290	-115.254	68.391
388.36	75.584	138.185	120.807	6.749	-118.306	-115.086	64.764
388.36	75.584	138.185	120.807	6.749	-120.371	-115.086	64.764
400	75.770	140.420	121.345	7.630	-120.475	-114.927	62.792
432.02	76.282	146.274	122.974	10.066	-120.859	-114.469	57.907
450	76.570	149.390	123.968	11.440	-121.452	-114.197	55.461
500	77.370	157.500	126.920	15.290	-122.242	-113.344	49.542
550	78.170	164.910	130.037	19.180	-122.936	-112.426	44.673

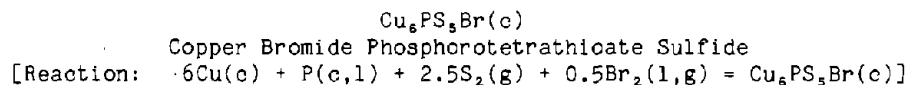
Phase changes: 317.3 K, melting point of P; $\Delta\text{H}^\circ = 0.157$ kcal/mol.
332.6 K, boiling point of Br; $\Delta\text{H}^\circ = 7.065$ kcal/mol.
368.3 K, orthorhombic - monoclinic transition point of S; $\Delta\text{H}^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta\text{H}^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta\text{H}^\circ = 0$ kcal/mol.

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

298.15-550 K: $\text{Cp}^\circ = 69.367 + 16.014 \times 10^{-3} \text{T}$
 $\text{H}^\circ - \text{H}_{298}^\circ = 69.367 \times 10^{-3} \text{T} + 8.007 \times 10^{-6} \text{T}^2 - 21.394$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta\text{Hf}^\circ = -107.445 - 16.267 \times 10^{-3} \text{T} + 8.597 \times 10^{-6} \text{T}^2 - 736.000 \text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -107.445 + 16.267 \times 10^{-3} \text{T} \ln \text{T} - 8.597 \times 10^{-6} \text{T}^2 - 368.000 \text{T}^{-1} - 112.508 \times 10^{-3} \text{T}$
317.3-332.6 K: $\Delta\text{Hf}^\circ = -107.132 - 18.761 \times 10^{-3} \text{T} + 11.782 \times 10^{-6} \text{T}^2 - 736.000 \text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -107.132 + 18.761 \times 10^{-3} \text{T} \ln \text{T} - 11.782 \times 10^{-6} \text{T}^2 - 368.000 \text{T}^{-1} - 126.844 \times 10^{-3} \text{T}$
332.6-368.3 K: $\Delta\text{Hf}^\circ = -112.132 - 14.180 \times 10^{-3} \text{T} + 11.705 \times 10^{-6} \text{T}^2 - 751.700 \text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -112.132 + 14.180 \times 10^{-3} \text{T} \ln \text{T} - 11.705 \times 10^{-6} \text{T}^2 - 375.850 \text{T}^{-1} - 85.167 \times 10^{-3} \text{T}$
368.3-388.36 K: $\Delta\text{Hf}^\circ = -117.708 - 2.865 \times 10^{-3} \text{T} + 2.975 \times 10^{-6} \text{T}^2 + 26.300 \text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -117.708 + 2.865 \times 10^{-3} \text{T} \ln \text{T} - 2.975 \times 10^{-6} \text{T}^2 + 13.150 \text{T}^{-1} - 9.252 \times 10^{-3} \text{T}$
388.36-432.02 K: $\Delta\text{Hf}^\circ = -198.499 + 220.835 \times 10^{-3} \text{T} - 213.436 \times 10^{-6} \text{T}^2 + 9537.300 \text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -198.499 - 220.835 \times 10^{-3} \text{T} \ln \text{T} + 213.436 \times 10^{-6} \text{T}^2 + 4768.650 \text{T}^{-1} + 1416.890 \times 10^{-3} \text{T}$
432.02-550 K: $\Delta\text{Hf}^\circ = -245.893 + 201.305 \times 10^{-3} \text{T} - 114.376 \times 10^{-6} \text{T}^2 + 25669.800 \text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -245.893 - 201.305 \times 10^{-3} \text{T} \ln \text{T} + 114.376 \times 10^{-6} \text{T}^2 + 12834.900 \text{T}^{-1} + 1407.652 \times 10^{-3} \text{T}$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	74.170	118.400	118.400	0	-190.775	-162.922	119.424
300	74.200	118.860	118.400	.140	-190.764	-162.745	118.558
317.3	74.466	123.028	118.533	1.426	-190.679	-161.131	110.982
317.3	74.466	123.028	118.533	1.426	-190.836	-161.131	110.982
332.6	74.702	126.534	118.843	2.558	-190.780	-159.708	104.942
332.6	74.702	126.534	118.843	2.558	-194.312	-159.708	104.942
350	74.970	130.350	119.321	3.860	-194.164	-157.904	98.598
400	75.770	140.420	121.345	7.630	-193.730	-152.755	83.460
450	76.570	149.390	123.968	11.440	-193.307	-147.661	71.713
500	77.370	157.500	126.920	15.290	-192.879	-142.611	62.334
550	78.170	164.910	130.037	19.180	-192.449	-137.614	54.682

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
332.6 K, boiling point of Br; ΔH° = 7.065 kcal/mol.

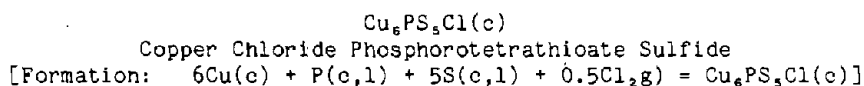
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: Cp° = 69.367 + 16.014x10⁻³T
H°- H₂₉₈° = 69.367x10⁻³T + 8.007x10⁻⁶T² - 21.394

Reaction equations (kcal/mol):

298.15-317.3 K: ΔHr° = -191.390 + 3.745x10⁻³T - 0.788x10⁻⁶T² - 128.750T⁻¹
ΔGr° = -191.390 - 3.745x10⁻³TlnT + 0.788x10⁻⁶T² - 64.375T⁻¹ + 117.307x10⁻³T
317.3-332.6 K: ΔHr° = -191.076 + 1.252x10⁻³T + 2.397x10⁻⁶T² - 128.750T⁻¹
ΔGr° = -191.076 - 1.252x10⁻³TlnT - 2.397x10⁻⁶T² - 64.375T⁻¹ + 102.971x10⁻³T
332.6-550 K: ΔHr° = -196.077 + 5.832x10⁻³T + 2.319x10⁻⁶T² - 144.450T⁻¹
ΔGr° = -196.077 - 5.832x10⁻³TlnT - 2.319x10⁻⁶T² - 72.225T⁻¹ + 144.648x10⁻³T

Source: Data based on Flechter (39).



T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	75.980	119.500	119.500	0	-122.000	-121.161	88.812
300	76.000	119.940	119.500	.140	-121.994	-121.147	88.254
317.3	76.325	124.210	119.616	1.458	-121.929	-121.099	83.409
317.3	76.325	124.210	119.616	1.458	-122.086	-121.099	83.409
350	76.940	131.790	120.447	3.970	-121.995	-121.018	75.566
368.3	77.149	135.717	121.109	5.380	-121.956	-120.968	71.782
368.3	77.149	135.717	121.109	5.380	-122.436	-120.968	71.782
388.36	77.377	139.813	121.972	6.929	-122.413	-120.886	68.028
388.36	77.377	139.813	121.972	6.929	-124.478	-120.886	68.028
400	77.510	142.100	122.525	7.830	-124.560	-120.779	65.989
432.02	77.875	148.080	124.197	10.318	-124.887	-120.465	60.940
450	78.080	151.260	125.216	11.720	-125.449	-120.275	58.413
500	78.640	159.520	128.240	15.640	-126.162	-119.659	52.302
550	79.210	167.040	131.422	19.590	-126.791	-118.981	47.278

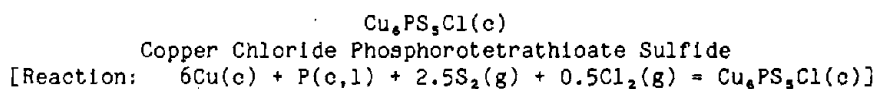
Phase changes: 317.3 K, melting point of P; $\Delta H^\circ = 0.157$ kcal/mol.
368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.

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

298.15-550 K: $C_p^\circ = 72.954 + 11.382 \times 10^{-3} T$
 $H^\circ - H_{298}^\circ = 72.954 \times 10^{-3} T + 5.691 \times 10^{-6} T^2 - 22.257$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta H_f^\circ = -117.567 - 8.049 \times 10^{-3} T + 6.187 \times 10^{-6} T^2 - 770.150 T^{-1}$
 $\Delta G_f^\circ = -117.567 + 8.049 \times 10^{-3} T \ln T - 6.187 \times 10^{-6} T^2 - 385.075 T^{-1} - 51.734 \times 10^{-3} T$
317.3-368.3 K: $\Delta H_f^\circ = -117.254 - 10.542 \times 10^{-3} T + 9.372 \times 10^{-6} T^2 - 770.150 T^{-1}$
 $\Delta G_f^\circ = -117.254 + 10.542 \times 10^{-3} T \ln T - 9.372 \times 10^{-6} T^2 - 385.075 T^{-1} - 66.071 \times 10^{-3} T$
368.3-388.36 K: $\Delta H_f^\circ = -122.829 + 0.773 \times 10^{-3} T + 0.642 \times 10^{-6} T^2 + 7.850 T^{-1}$
 $\Delta G_f^\circ = -122.829 - 0.773 \times 10^{-3} T \ln T - 0.642 \times 10^{-6} T^2 + 3.925 T^{-1} + 9.844 \times 10^{-3} T$
388.36-432.02 K: $\Delta H_f^\circ = -203.621 + 224.473 \times 10^{-3} T - 215.768 \times 10^{-6} T^2 + 9518.850 T^{-1}$
 $\Delta G_f^\circ = -203.621 - 224.473 \times 10^{-3} T \ln T + 215.768 \times 10^{-6} T^2 + 4759.425 T^{-1} + 1435.986 \times 10^{-3} T$
432.02-550 K: $\Delta H_f^\circ = -251.014 + 204.944 \times 10^{-3} T - 116.708 \times 10^{-6} T^2 + 25651.350 T^{-1}$
 $\Delta G_f^\circ = -251.014 - 204.944 \times 10^{-3} T \ln T + 116.708 \times 10^{-6} T^2 + 12825.675 T^{-1} + 1426.749 \times 10^{-3} T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHr°	ΔGr°	
298.15	75.980	119.500	119.500	0	-198.775	-168.729	123.680
300	76.000	119.940	119.500	.140	-198.755	-168.533	122.775
317.3	76.325	124.210	119.616	1.458	-198.552	-166.795	114.883
317.3	76.325	124.210	119.616	1.458	-198.709	-166.795	114.883
350	76.940	131.790	120.447	3.970	-198.349	-163.542	102.119
400	77.510	142.100	122.525	7.830	-197.814	-158.606	86.657
450	78.080	151.260	125.216	11.720	-197.304	-153.739	74.665
500	78.640	159.520	128.240	15.640	-196.799	-148.925	65.094
550	79.210	167.040	131.422	19.590	-196.305	-144.169	57.287

Phase change: 317.3 K, melting point of P; $\Delta\text{H}^\circ = 0.157$ kcal/mol.

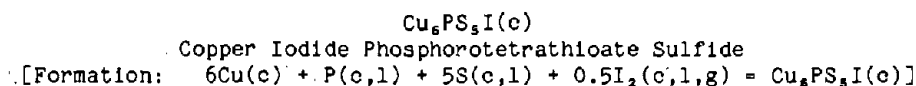
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-550 K: $\text{Cp}^\circ = 72.954 + 11.382 \times 10^{-3} \text{T}$
 $\text{H}^\circ - \text{H}_{298}^\circ = 72.954 \times 10^{-3} \text{T} + 5.691 \times 10^{-6} \text{T}^2 - 22.257$

Reaction equations (kcal/mol):

298.15-317.3 K: $\Delta\text{Hr}^\circ = -201.511 + 11.964 \times 10^{-3} \text{T} - 3.198 \times 10^{-6} \text{T}^2 - 162.900 \text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -201.511 - 11.964 \times 10^{-3} \text{T} \ln \text{T} + 3.198 \times 10^{-6} \text{T}^2 - 81.450 \text{T}^{-1} + 178.081 \times 10^{-3} \text{T}$
 317.3-550 K: $\Delta\text{Hr}^\circ = -201.198 + 9.471 \times 10^{-3} \text{T} - 0.013 \times 10^{-6} \text{T}^2 - 162.900 \text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -201.198 - 9.471 \times 10^{-3} \text{T} \ln \text{T} + 0.013 \times 10^{-6} \text{T}^2 - 81.450 \text{T}^{-1} + 163.744 \times 10^{-3} \text{T}$

Source: Data based on Flechter (39).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	74.210	119.050	119.050	0	-105.000	-107.833	79.043
300	74.230	119.510	119.050	.140	-104.999	-107.847	78.566
317.3	74.403	123.677	119.183	1.426	-105.009	-108.010	74.394
317.3	74.403	123.677	119.183	1.426	-105.166	-108.010	74.394
350	74.730	130.990	119.961	3.860	-105.237	-108.305	67.628
368.3	74.913	134.803	120.605	5.229	-105.295	-108.464	64.362
368.3	74.913	134.803	120.605	5.229	-105.775	-108.464	64.362
386.8	75.098	138.478	121.369	6.618	-105.854	-108.592	61.356
386.8	75.098	138.478	121.369	6.618	-107.708	-108.592	61.356
388.36	75.114	138.780	121.438	6.735	-107.719	-108.595	61.111
388.36	75.114	138.780	121.438	6.735	-109.784	-108.595	61.111
400	75.230	141.000	121.975	7.610	-109.955	-108.559	59.313
432.02	75.544	146.806	123.612	10.020	-110.533	-108.431	54.852
450	75.720	149.890	124.601	11.380	-111.234	-108.334	52.614
458.4	75.804	151.291	125.077	12.016	-111.528	-108.278	51.623
458.4	75.804	151.291	125.077	12.016	-116.539	-108.278	51.623
500	76.220	157.890	127.530	15.180	-117.130	-107.501	46.988
550	76.720	165.180	130.616	19.010	-117.887	-106.504	42.320

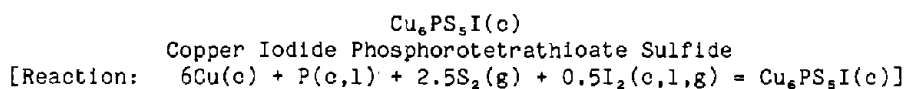
Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
386.8 K, melting point of I₂; ΔH° = 3.709 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
458.4 K, boiling point of I₂; ΔH° = 10.021 kcal/mol.

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

298.15-550 K: Cp° = 71.243 + 9.960x10⁻³T
H° - H₂₉₈° = 71.243x10⁻³T + 4.980x10⁻⁶T² - 21.684

Formation equations (kcal/mol):

298.15-317.3 K: ΔHf° = -99.442 - 11.785x10⁻³T + 4.774x10⁻⁶T² - 736.000T⁻¹
ΔGf° = -99.442 + 11.785x10⁻³TlnT - 4.774x10⁻⁶T² - 368.000T⁻¹ - 89.723x10⁻³T
317.3-368.3 K: ΔHf° = -99.129 - 14.278x10⁻³T + 7.959x10⁻⁶T² - 736.000T⁻¹
ΔGf° = -99.129 + 14.278x10⁻³TlnT - 7.959x10⁻⁶T² - 368.000T⁻¹ - 104.059x10⁻³T
368.3-386.8 K: ΔHf° = -104.704 - 2.963x10⁻³T - 0.771x10⁻⁶T² + 42.000T⁻¹
ΔGf° = -104.704 + 2.963x10⁻³TlnT + 0.771x10⁻⁶T² + 21.000T⁻¹ - 28.145x10⁻³T
386.8-388.36 K: ΔHf° = -105.432 - 6.165x10⁻³T - 0.025x10⁻⁶T² + 42.000T⁻¹
ΔGf° = -105.432 + 6.165x10⁻³TlnT + 0.025x10⁻⁶T² + 21.000T⁻¹ - 45.052x10⁻³T
388.36-432.02 K: ΔHf° = -186.224 + 217.535x10⁻³T - 216.435x10⁻⁶T² + 9553.000T⁻¹
ΔGf° = -186.224 + 217.535x10⁻³TlnT + 216.435x10⁻⁶T² + 4776.500T⁻¹ + 1381.090x10⁻³T
432.02-458.4 K: ΔHf° = -233.617 + 198.006x10⁻³T - 117.375x10⁻⁶T² + 25685.500T⁻¹
ΔGf° = -233.617 - 198.006x10⁻³TlnT + 117.375x10⁻⁶T² + 12842.750T⁻¹ + 1371.852x10⁻³T
458.4-550 K: ΔHf° = -240.974 + 203.176x10⁻³T - 117.409x10⁻⁶T² + 25677.850T⁻¹
ΔGf° = -240.974 - 203.176x10⁻³TlnT + 117.409x10⁻⁶T² + 12838.925T⁻¹ + 1419.584x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	74.210	119.050	119.050	0	-181.775	-155.401	113.911
300	74.230	119.510	119.050	.140	-181.759	-155.234	113.086
317.3	74.403	123.677	119.183	1.426	-181.633	-153.707	105.869
317.3	74.403	123.677	119.183	1.426	-181.790	-153.707	105.869
350	74.730	130.990	119.961	3.860	-181.591	-150.829	94.181
386.8	75.098	138.478	121.369	6.618	-181.392	-147.602	83.397
386.8	75.098	138.478	121.369	6.618	-183.247	-147.602	83.397
400	75.230	141.000	121.975	7.610	-183.210	-146.387	79.981
450	75.720	149.890	124.601	11.380	-183.089	-141.798	68.866
458.4	75.804	151.291	125.077	12.016	-183.069	-141.028	67.236
458.4	75.804	151.291	125.077	12.016	-188.079	-141.028	67.236
500	76.220	157.890	127.530	15.180	-187.768	-136.767	59.780
550	76.720	165.180	130.616	19.010	-187.400	-131.692	52.329

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
386.8 K, melting point of I₂; ΔH° = 3.709 kcal/mol.
458.4 K, boiling point of I₂; ΔH° = 10.021 kcal/mol.

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

298.15-550 K: Cp° = 71.243 + 9.960x10⁻³T
H° - H°₂₉₈ = 71.243x10⁻³T + 4.980x10⁻⁶T² - 21.684

Reaction equations (kcal/mol):

298.15-317.3 K: ΔHr° = -183.386 + 8.228x10⁻³T - 4.611x10⁻⁶T² - 128.750T⁻¹
ΔGr° = -183.386 - 8.228x10⁻³TlnT + 4.611x10⁻⁶T² - 64.375T⁻¹ + 140.092x10⁻³T
317.3-386.8 K: ΔHr° = -183.073 + 5.735x10⁻³T - 1.426x10⁻⁶T² - 128.750T⁻¹
ΔGr° = -183.073 - 5.735x10⁻³TlnT + 1.426x10⁻⁶T² - 64.375T⁻¹ + 125.756x10⁻³T
386.8-458.4 K: ΔHr° = -183.801 + 2.533x10⁻³T - 0.680x10⁻⁶T² - 128.750T⁻¹
ΔGr° = -183.801 - 2.533x10⁻³TlnT + 0.680x10⁻⁶T² - 64.375T⁻¹ + 108.848x10⁻³T
458.4-550 K: ΔHr° = -191.157 + 7.703x10⁻³T - 0.714x10⁻⁶T² - 136.400T⁻¹
ΔGr° = -191.157 - 7.703x10⁻³TlnT + 0.714x10⁻⁶T² - 68.200T⁻¹ + 156.580x10⁻³T

Source: Data based on Fiechter (39).

CuS(c)
Copper Monosulfide
[Formation: Cu(c) + S(c,1) = CuS(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	11.324	16.053	16.053	0	-13.300	-13.440	9.851
300	11.339	16.124	16.054	.021	-13.300	-13.440	9.791
368.3	11.803	18.505	16.293	.814	-13.294	-13.473	7.995
368.3	11.803	18.505	16.293	.814	-13.390	-13.473	7.995
388.36	11.939	19.134	16.424	1.053	-13.391	-13.477	7.584
388.36	11.939	19.134	16.424	1.053	-13.804	-13.477	7.584
400	12.018	19.488	16.508	1.192	-13.823	-13.467	7.358
432.02	12.199	20.420	16.764	1.580	-13.892	-13.436	6.797
500	12.582	22.231	17.387	2.422	-14.142	-13.343	5.832
600	13.100	24.571	18.393	3.707	-14.340	-13.161	4.794
700	13.595	26.628	19.425	5.042	-14.444	-12.955	4.045
717.824	13.683	26.971	19.608	5.285	-14.453	-12.917	3.933

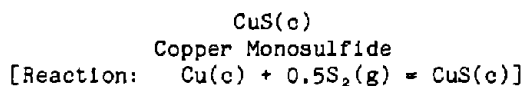
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-780 K: $C_p^\circ = 10.290 + 4.840 \times 10^{-3}T - 0.330 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 10.290 \times 10^{-3}T + 2.420 \times 10^{-6}T^2 + 0.330 \times 10^{-2}T^{-1} - 3.394$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -12.253 - 3.204 \times 10^{-3}T + 3.327 \times 10^{-6}T^2 - 115.600T^{-1}$
 $\Delta G_f^\circ = -12.253 + 3.204 \times 10^{-3}T \ln T - 3.327 \times 10^{-6}T^2 - 57.800T^{-1} - 20.593 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -13.368 - 0.941 \times 10^{-3}T + 1.581 \times 10^{-6}T^2 + 40 T^{-1}$
 $\Delta G_f^\circ = -13.368 + 0.941 \times 10^{-3}T \ln T - 1.581 \times 10^{-6}T^2 + 20 T^{-1} - 5.410 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -29.526 + 43.799 \times 10^{-3}T - 41.701 \times 10^{-6}T^2 + 1942.200T^{-1}$
 $\Delta G_f^\circ = -29.526 - 43.799 \times 10^{-3}T \ln T + 41.701 \times 10^{-6}T^2 + 971.100T^{-1} + 279.818 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -39.005 + 39.893 \times 10^{-3}T - 21.889 \times 10^{-6}T^2 + 5168.700T^{-1}$
 $\Delta G_f^\circ = -39.005 - 39.893 \times 10^{-3}T \ln T + 21.889 \times 10^{-6}T^2 + 2584.350T^{-1} + 277.970 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	11.324	16.053	16.053	0	-28.655	-22.953	16.825
300	11.339	16.124	16.054	.021	-28.652	-22.918	16.695
400	12.018	19.488	16.508	1.192	-28.474	-21.033	11.492
500	12.582	22.231	17.387	2.422	-28.270	-19.196	8.391
600	13.100	24.571	18.393	3.707	-28.035	-17.402	6.339
700	13.595	26.628	19.425	5.042	-27.769	-15.650	4.886
780	13.989	28.120	20.242	6.145	-27.534	-14.278	4.001

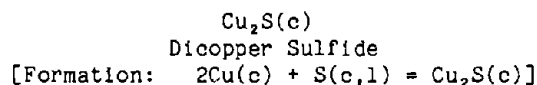
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-780 K: $\text{Cp}^\circ = 10.290 + 4.840 \times 10^{-3}T - 0.330 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 10.290 \times 10^{-3}T + 2.420 \times 10^{-6}T^2 + 0.330 \times 10^{-2}T^{-1} - 3.394$

Reaction equations (kcal/mol):

298.15-780 K: $\Delta \text{Hr}^\circ = -29.042 + 0.798 \times 10^{-3}T + 1.450 \times 10^{-6}T^2 + 5.850T^{-1}$
 $\Delta \text{Gr}^\circ = -29.042 - 0.798 \times 10^{-3}T \ln T - 1.450 \times 10^{-6}T^2 + 2.925T^{-1} + 25.370 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Stuve (112). Other data from Ferrante (37).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	18.382	27.761	27.761	0	-18.100	-19.368	14.197
300	18.420	27.875	27.762	.034	-18.098	-19.375	14.115
368.3	20.011	31.794	28.150	1.342	-17.981	-19.676	11.676
368.3	20.011	31.794	28.150	1.342	-18.077	-19.676	11.676
376	20.190	32.210	28.228	1.497	-18.060	-19.710	11.456
376	23.960	34.510	28.228	2.362	-17.195	-19.710	11.456
388.36	23.831	35.288	28.446	2.657	-17.122	-19.794	11.139
388.36	23.831	35.288	28.446	2.657	-17.535	-19.794	11.139
400	23.710	35.990	28.655	2.934	-17.486	-19.863	10.853
432.02	23.406	37.804	29.267	3.688	-17.382	-20.058	10.147
500	22.760	41.180	30.666	5.257	-17.324	-20.484	8.953
600	21.930	45.250	32.767	7.490	-17.200	-21.124	7.694
700	21.210	48.580	34.800	9.646	-17.122	-21.788	6.802
717.824	21.103	49.106	35.142	10.024	-17.111	-21.901	6.668

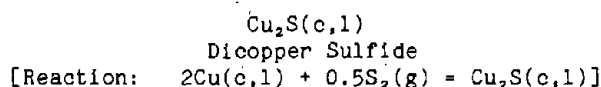
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 376 K, α - β transition point of Cu₂S; ΔH° = 0.865 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-376 K: Cp° = 5.240 + 35.440x10⁻³T + 2.290x10⁻⁵T⁻²
 H°- H₂₉₈° = 5.240x10⁻³T + 17.720x10⁻⁶T² - 2.290x10⁻²T⁻¹ - 2.369
 376-720 K: Cp° = 25.241 - 6.240x10⁻³T + 1.580x10⁻⁵T⁻²
 H°- H₂₉₈° = 25.241x10⁻³T - 3.120x10⁻⁶T² - 1.580x10⁻²T⁻¹ - 6.267

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -14.394 - 13.574x10⁻³T + 17.817x10⁻⁶T² - 370.600T⁻¹
 ΔGf° = -14.394 + 13.574x10⁻³TlnT - 17.817x10⁻⁶T² - 185.300T⁻¹ - 86.625x10⁻³T
 368.3-376 K: ΔHf° = -15.509 - 11.311x10⁻³T + 16.071x10⁻⁶T² - 215.000T⁻¹
 ΔGf° = -15.509 + 11.311x10⁻³TlnT - 16.071x10⁻⁶T² - 107.500T⁻¹ - 71.442x10⁻³T
 376-388.36 K: ΔHf° = -19.407 + 8.690x10⁻³T - 4.769x10⁻⁶T² - 144.000T⁻¹
 ΔGf° = -19.407 - 8.690x10⁻³TlnT + 4.769x10⁻⁶T² - 72.000T⁻¹ + 49.435x10⁻³T
 388.36-432.02 K: ΔHf° = -35.565 + 53.430x10⁻³T - 48.051x10⁻⁶T² + 1758.200T⁻¹
 ΔGf° = -35.565 - 53.430x10⁻³TlnT + 48.051x10⁻⁶T² + 879.100T⁻¹ + 334.663x10⁻³T
 432.02-717.824 K: ΔHf° = -45.044 + 49.524x10⁻³T - 28.239x10⁻⁶T² + 4984.700T⁻¹
 ΔGf° = -45.044 - 49.524x10⁻³TlnT + 28.239x10⁻⁶T² + 2492.350T⁻¹ + 332.816x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	18.382	27.761	27.761	0	-33.455	-28.881	21.170
300	18.420	27.875	27.762	.034	-33.450	-28.853	21.019
376	20.190	32.210	28.228	1.497	-33.188	-27.715	16.109
376	23.960	34.510	28.228	2.362	-32.323	-27.715	16.109
400	23.710	35.990	28.655	2.934	-32.137	-27.429	14.986
500	22.760	41.180	30.666	5.257	-31.451	-26.337	11.512
600	21.930	45.250	32.767	7.490	-30.895	-25.365	9.239
700	21.210	48.580	34.800	9.646	-30.447	-24.483	7.644
720	21.090	49.170	35.184	10.070	-30.368	-24.309	7.379
720	19.830	49.560	35.184	10.350	-30.088	-24.309	7.379
800	19.770	51.650	36.731	11.935	-29.896	-23.680	6.469
900	19.700	53.970	38.520	13.905	-29.692	-22.915	5.565
1000	19.620	56.040	40.165	15.875	-29.517	-22.167	4.844
1100	19.550	57.910	41.701	17.830	-29.394	-21.444	4.260
1200	19.480	59.610	43.123	19.785	-29.320	-20.723	3.774
1300	19.410	61.160	44.445	21.730	-29.321	-20.001	3.362
1357.6	19.364	62.005	45.178	22.845	-29.370	-19.600	3.155
1357.6	19.364	62.005	45.178	22.845	-35.610	-19.600	3.155
1400	19.330	62.600	45.696	23.665	-35.647	-19.100	2.982
1400	21.430	64.790	45.694	26.735	-32.577	-19.096	2.981
1500	21.430	66.270	47.017	28.880	-32.454	-18.138	2.643
1600	21.430	67.650	48.259	31.025	-32.334	-17.179	2.346

Phase changes: 376 K, α - β transition point of Cu₂S; ΔH° = 0.865 kcal/mol.
720 K, β - γ transition point of Cu₂S; ΔH° = 0.280 kcal/mol.
1357.6 K, melting point of Cu; ΔH° = 3.120 kcal/mol.
1400 K, melting point of Cu₂S; ΔH° = 3.070 kcal/mol.

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

298.15-376 K: Cp° = 5.240 + 35.440x10⁻³T + 2.290x10⁻⁵T⁻²
H° - H₂₉₈° = 5.240x10⁻³T + 17.720x10⁻⁶T² - 2.290x10⁻²T⁻¹ - 2.369
376-720 K: Cp° = 25.241 - 6.240x10⁻³T + 1.580x10⁻⁵T⁻²
H° - H₂₉₈° = 25.241x10⁻³T - 3.120x10⁻⁶T² - 1.580x10⁻²T⁻¹ - 6.267
720-1400 K: Cp° = 20.380 - 0.740x10⁻³T - 0.153x10⁻⁵T⁻²
H° - H₂₉₈° = 20.380x10⁻³T - 0.370x10⁻⁶T² + 0.153x10⁻²T⁻¹ - 4.153
1400-1600 K: Cp° = 21.430
H° - H₂₉₈° = 21.430x10⁻³T - 3.267

Reaction equations (kcal/mol):

298.15-376 K: ΔHr° = -31.183 - 9.571x10⁻³T + 15.940x10⁻⁶T² - 249.150T⁻¹
ΔGr° = -31.183 + 9.571x10⁻³T lnT - 15.940x10⁻⁶T² - 124.575T⁻¹ - 40.662x10⁻³T
376-720 K: ΔHr° = -35.080 + 10.429x10⁻³T - 4.900x10⁻⁶T² - 178.150T⁻¹
ΔGr° = -35.080 - 10.429x10⁻³T lnT + 4.900x10⁻⁶T² - 89.075T⁻¹ + 80.215x10⁻³T
720-1357.6 K: ΔHr° = -32.967 + 5.568x10⁻³T - 2.150x10⁻⁶T² - 4.850T⁻¹
ΔGr° = -32.967 - 5.568x10⁻³T lnT + 2.150x10⁻⁶T² - 2.425T⁻¹ + 47.111x10⁻³T
1357.6-1400 K: ΔHr° = -35.449 + 0.608x10⁻³T - 0.530x10⁻⁶T² - 18.850T⁻¹
ΔGr° = -35.449 - 0.608x10⁻³T lnT + 0.530x10⁻⁶T² - 9.425T⁻¹ + 15.363x10⁻³T
1400-1600 K: ΔHr° = -34.563 + 1.658x10⁻³T - 0.160x10⁻⁶T² - 34.150T⁻¹
ΔGr° = -34.563 - 1.658x10⁻³T lnT + 0.160x10⁻⁶T² - 17.075T⁻¹ + 22.859x10⁻³T

Sources: Enthalpy of formation at 298 K from Stuve (112). Other data from Ferrante (37).

DyS(g)
Dysprosium Monosulfide (ideal gas)
[Formation: Dy(c) + S(c,l) = DyS(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15*	8.200	63.520	63.520	0	39.000	27.683	-20.292
300	8.210	63.570	63.520	.015	38.993	27.612	-20.115
368.3	8.415	65.281	63.694	.585	38.719	25.048	-14.863
368.3	8.415	65.281	63.694	.585	38.623	25.048	-14.863
388.36	8.475	65.729	63.787	.754	38.539	24.312	-13.681
388.36	8.475	65.729	63.787	.754	38.126	24.312	-13.681
400	8.510	65.980	63.848	.853	38.059	23.899	-13.057
432.02	8.555	66.637	64.030	1.126	37.854	22.772	-11.520
500	8.650	67.890	64.466	1.712	37.309	20.448	-8.937
600	8.730	69.480	65.178	2.581	36.646	17.135	-6.241
700	8.780	70.830	65.893	3.456	36.038	13.936	-4.351
717.824	8.785	71.051	66.018	3.613	35.934	13.375	-4.072

*Data except enthalpy of formation at 298 K estimated.

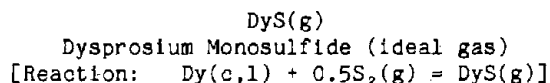
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 8.875 + 0.036x10⁻³T - 0.608x10⁻⁵T⁻²
H° - H₂₉₈° = 8.875x10⁻³T + 0.018x10⁻⁶T² + 0.608x10⁻²T⁻¹ - 2.852

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 39.626 - 2.789x10⁻³T - 0.490x10⁻⁶T² + 74.400T⁻¹
ΔGf° = 39.626 + 2.789x10⁻³TlnT + 0.490x10⁻⁶T² + 37.200T⁻¹ - 56.512x10⁻³T
368.3-388.36 K: ΔHf° = 38.510 - 0.526x10⁻³T - 2.236x10⁻⁶T² + 230 T⁻¹
ΔGf° = 38.510 + 0.526x10⁻³TlnT + 2.236x10⁻⁶T² + 115.000T⁻¹ - 41.329x10⁻³T
388.36-432.02 K: ΔHf° = 22.352 + 44.214x10⁻³T - 45.518x10⁻⁶T² + 2132.200T⁻¹
ΔGf° = 22.352 - 44.214x10⁻³TlnT + 45.518x10⁻⁶T² + 1066.100T⁻¹ + 243.899x10⁻³T
432.02-717.824 K: ΔHf° = 12.873 + 40.308x10⁻³T - 25.706x10⁻⁶T² + 5358.700T⁻¹
ΔGf° = 12.873 - 40.308x10⁻³TlnT + 25.706x10⁻⁶T² + 2679.350T⁻¹ + 242.052x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	8.200	63.520	63.520	0	23.645	18.169	-13.318
300	8.210	63.570	63.520	.015	23.641	18.135	-13.211
400	8.510	65.980	63.848	.853	23.408	16.333	-8.924
500	8.650	67.890	64.466	1.712	23.182	14.594	-6.379
600	8.730	69.480	65.178	2.581	22.952	12.894	-4.697
700	8.780	70.830	65.893	3.456	22.713	11.241	-3.510
800	8.810	72.000	66.580	4.336	22.458	9.621	-2.628
900	8.830	73.040	67.242	5.218	22.182	8.035	-1.951
1000	8.850	73.970	67.868	6.102	21.879	6.478	-1.416
1100	8.860	74.820	68.467	6.988	21.539	4.946	-.983
1200	8.880	75.590	69.027	7.875	21.149	3.458	-.630
1300	8.890	76.300	69.559	8.763	20.696	2.003	-.337
1400	8.890	76.960	70.066	9.652	20.175	.577	-.090
1500	8.900	77.570	70.542	10.542	19.577	-.793	.116
1600	8.910	78.150	71.005	11.432	18.895	-2.145	.293
1657	8.910	78.462	71.256	11.940	18.466	-2.872	.379
1657	8.910	78.462	71.256	11.940	17.471	-2.872	.379
1682	8.910	78.595	71.364	12.163	17.410	-3.180	.413
1682	8.910	78.595	71.364	12.163	14.767	-3.180	.413
1700	8.910	78.690	71.441	12.323	14.629	-3.384	.435
1800	8.920	79.200	71.858	13.215	13.855	-4.406	.535
1900	8.930	79.680	72.255	14.108	13.080	-5.404	.622
2000	8.930	80.140	72.640	15.000	12.300	-6.366	.696

*Data except enthalpy of formation at 298 K estimated.

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: $C_p^\circ = 8.875 + 0.036 \times 10^{-3}T - 0.608 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 8.875 \times 10^{-3}T + 0.018 \times 10^{-6}T^2 + 0.608 \times 10^{-2}T^{-1} - 2.852$

Reaction equations (kcal/mol):

298.15-1657 K: $\Delta H_r^\circ = 22.837 + 1.214 \times 10^{-3}T - 2.367 \times 10^{-6}T^2 + 195.850T^{-1}$
 $\Delta G_r^\circ = 22.837 - 1.214 \times 10^{-3}T \ln T + 2.367 \times 10^{-6}T^2 + 97.925T^{-1} - 10.549 \times 10^{-3}T$
1657-1682 K: $\Delta H_r^\circ = 21.154 - 1.996 \times 10^{-3}T - 0.142 \times 10^{-6}T^2 + 26.650T^{-1}$
 $\Delta G_r^\circ = 21.154 + 1.996 \times 10^{-3}T \ln T + 0.142 \times 10^{-6}T^2 + 13.325T^{-1} - 29.611 \times 10^{-3}T$
1682-2000 K: $\Delta H_r^\circ = 27.308 - 7.226 \times 10^{-3}T - 0.142 \times 10^{-6}T^2 + 26.650T^{-1}$
 $\Delta G_r^\circ = 27.308 + 7.226 \times 10^{-3}T \ln T + 0.142 \times 10^{-6}T^2 + 13.325T^{-1} - 72.117 \times 10^{-3}T$

Source: Data from Mills (80) who estimated all except enthalpy of formation at 298 K.

ErS(g)
Erbium Monosulfide (ideal gas)
[Formation: Er(c) + S(c,l) = ErS(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15*	8.200	62.580	62.580	0	49.000	37.841	-27.738
300	8.210	62.630	62.580	.015	48.993	37.771	-27.516
368.3	8.415	64.341	62.754	.585	48.718	35.247	-20.915
368.3	8.415	64.341	62.754	.585	48.622	35.247	-20.915
388.36	8.475	64.789	62.847	.754	48.536	34.522	-19.427
388.36	8.475	64.789	62.847	.754	48.123	34.522	-19.427
400	8.510	65.040	62.908	.853	48.055	34.115	-18.639
432.02	8.555	65.697	63.090	1.126	47.847	33.006	-16.697
500	8.650	66.950	63.526	1.712	47.294	30.718	-13.426
600	8.730	68.540	64.238	2.581	46.614	27.463	-10.003
700	8.780	69.890	64.953	3.456	45.985	24.324	-7.594
717.824	8.785	70.111	65.078	3.613	45.878	23.775	-7.238

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

$$298.15-2000^{\circ}\text{K:} \quad \text{Cp}^{\circ} = 8.875 + 0.036 \times 10^{-3}T - 0.608 \times 10^{-5}T^{-2}$$

$$\text{H}^{\circ} - \text{H}_{298}^{\circ} = 8.875 \times 10^{-3}T + 0.018 \times 10^{-6}T^2 + 0.608 \times 10^{-2}T^{-1} - 2.852$$

Formation equations (kcal/mol):

$$298.15-368.3 \text{ K:} \quad \Delta \text{Hf}^{\circ} = 50.439 - 4.579 \times 10^{-3}T + 0.476 \times 10^{-6}T^2 - 34.500T^{-1}$$

$$\Delta \text{Gf}^{\circ} = 50.439 + 4.579 \times 10^{-3}T \ln T - 0.476 \times 10^{-6}T^2 - 17.250T^{-1} - 68.008 \times 10^{-3}T$$

$$368.3-388.36 \text{ K:} \quad \Delta \text{Hf}^{\circ} = 49.324 - 2.316 \times 10^{-3}T - 1.270 \times 10^{-6}T^2 + 121.100T^{-1}$$

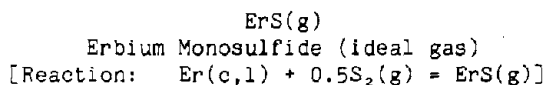
$$\Delta \text{Gf}^{\circ} = 49.324 + 2.316 \times 10^{-3}T \ln T + 1.270 \times 10^{-6}T^2 + 60.550T^{-1} - 52.825 \times 10^{-3}T$$

$$388.36-432.02 \text{ K:} \quad \Delta \text{Hf}^{\circ} = 33.165 + 42.424 \times 10^{-3}T - 44.552 \times 10^{-6}T^2 + 2023.300T^{-1}$$

$$\Delta \text{Gf}^{\circ} = 33.165 - 42.424 \times 10^{-3}T \ln T + 44.552 \times 10^{-6}T^2 + 1011.650T^{-1} + 232.404 \times 10^{-3}T$$

$$432.02-717.824 \text{ K:} \quad \Delta \text{Hf}^{\circ} = 23.687 + 38.518 \times 10^{-3}T - 24.740 \times 10^{-6}T^2 + 5249.800T^{-1}$$

$$\Delta \text{Gf}^{\circ} = 23.687 - 38.518 \times 10^{-3}T \ln T + 24.740 \times 10^{-6}T^2 + 2624.900T^{-1} + 230.556 \times 10^{-3}T$$



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15*	8.200	62.580	62.580	0	33.645	28.327	-20.764
300	8.210	62.630	62.580	.015	33.641	28.294	-20.612
400	8.510	65.040	62.908	.853	33.404	26.549	-14.506
500	8.650	66.950	63.526	1.712	33.167	24.864	-10.868
600	8.730	68.540	64.238	2.581	32.920	23.222	-8.459
700	8.780	69.890	64.953	3.456	32.660	21.629	-6.753
800	8.810	71.060	65.640	4.336	32.386	20.069	-5.483
900	8.830	72.100	66.302	5.218	32.092	18.548	-4.504
1000	8.850	73.030	66.928	6.102	31.777	17.066	-3.730
1100	8.860	73.880	67.527	6.988	31.436	15.602	-3.100
1200	8.880	74.650	68.088	7.875	31.069	14.181	-2.583
1300	8.890	75.360	68.619	8.763	30.670	12.796	-2.151
1400	8.890	76.020	69.126	9.652	30.236	11.436	-1.785
1500	8.900	76.630	69.602	10.542	29.768	10.103	-1.472
1600	8.910	77.210	70.065	11.432	29.260	8.812	-1.204
1700	8.910	77.750	70.501	12.323	28.711	7.553	-.971
1795	8.920	78.235	70.898	13.170	28.149	6.386	-.778
1795	8.920	78.235	70.898	13.170	23.392	6.386	-.778
1800	8.920	78.260	70.918	13.215	23.367	6.329	-.768
1900	8.930	78.740	71.315	14.108	22.858	5.400	-.621
2000	8.930	79.200	71.700	15.000	22.347	4.501*	-.492

*Data except enthalpy of formation at 298 K estimated.

Phase change: 1795 K, melting point of Er; $\Delta H^\circ = 4.757$ kcal/mol.

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

298.15-2000 K: $C_p^\circ = 8.875 + 0.036 \times 10^{-3}T - 0.608 \times 10^{-6}T^2$
 $H^\circ - H_{298}^\circ = 8.875 \times 10^{-3}T + 0.018 \times 10^{-6}T^2 + 0.608 \times 10^{-9}T^3 - 2.852$

Reaction equations (kcal/mol):

298.15-1795 K: $\Delta H_r^\circ = 33.650 - 0.576 \times 10^{-3}T - 1.401 \times 10^{-6}T^2 + 86.950T^{-1}$
 $\Delta G_r^\circ = 33.650 + 0.576 \times 10^{-3}T \ln T + 1.401 \times 10^{-6}T^2 + 43.475T^{-1} - 22.045 \times 10^{-3}T$
1795-2000 K: $\Delta H_r^\circ = 31.996 - 4.546 \times 10^{-3}T - 0.142 \times 10^{-6}T^2 + 26.650T^{-1}$
 $\Delta G_r^\circ = 31.996 + 4.546 \times 10^{-3}T \ln T + 0.142 \times 10^{-6}T^2 + 13.325T^{-1} - 48.600 \times 10^{-3}T$

Source: Data from Mills (80) who estimated all except enthalpy of formation at 298 K.

EuS(c)
Europium Monosulfide
[Formation: $\text{Eu(c)} + \text{S(c,l)} = \text{EuS(c)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	12.140	22.900	22.900	0	-109.700	-108.698	79.677
300	12.150	22.970	22.900	.022	-109.700	-108.690	79.180
368.3	12.369	25.495	23.153	.862	-109.697	-108.460	64.360
368.3	12.369	25.495	23.153	.862	-109.793	-108.460	64.360
388.36	12.433	26.152	23.291	1.111	-109.797	-108.387	60.994
388.36	12.433	26.152	23.291	1.111	-110.210	-108.387	60.994
400	12.470	26.520	23.380	1.256	-110.231	-108.332	59.189
432.02	12.508	27.482	23.649	1.656	-110.309	-108.177	54.724
500	12.590	29.320	24.300	2.510	-110.594	-107.816	47.126
600	12.670	31.620	25.332	3.773	-110.896	-107.229	39.058
700	12.750	33.580	26.373	5.045	-111.162	-106.596	33.280
717.824	12.768	33.901	26.556	5.272	-111.206	-106.479	32.418

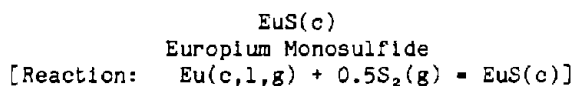
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $C_p^\circ = 11.173 + 2.236 \times 10^{-3}T + 0.267 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 11.173 \times 10^{-3}T + 1.118 \times 10^{-6}T^2 - 0.267 \times 10^{-2}T^{-1} - 3.341$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -109.035 - 1.297 \times 10^{-3}T + 0.555 \times 10^{-6}T^2 - 97.700T^{-1}$
 $\Delta G_f^\circ = -109.035 + 1.297 \times 10^{-3}T \ln T - 0.555 \times 10^{-6}T^2 - 48.850T^{-1} - 5.544 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -110.150 + 0.966 \times 10^{-3}T - 1.191 \times 10^{-6}T^2 + 57.900T^{-1}$
 $\Delta G_f^\circ = -110.150 - 0.966 \times 10^{-3}T \ln T + 1.191 \times 10^{-6}T^2 + 28.950T^{-1} + 9.639 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -126.308 + 45.706 \times 10^{-3}T - 44.473 \times 10^{-6}T^2 + 1960.100T^{-1}$
 $\Delta G_f^\circ = -126.308 - 45.706 \times 10^{-3}T \ln T + 44.473 \times 10^{-6}T^2 + 980.050T^{-1} + 294.867 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -135.787 + 41.800 \times 10^{-3}T - 24.661 \times 10^{-6}T^2 + 5186.600T^{-1}$
 $\Delta G_f^\circ = -135.787 - 41.800 \times 10^{-3}T \ln T + 24.661 \times 10^{-6}T^2 + 2593.300T^{-1} + 293.020 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°-H° ₂₉₈)/T	H°-H° ₂₉₈	ΔHr°	ΔGr°	
298.15	12.140	22.900	22.900	0	-125.055	-118.212	86.650
300	12.150	22.970	22.900	.022	-125.052	-118.167	86.084
400	12.470	26.520	23.380	1.256	-124.882	-115.897	63.323
500	12.590	29.320	24.300	2.510	-124.721	-113.670	49.684
600	12.670	31.620	25.332	3.773	-124.590	-111.470	40.603
700	12.750	33.580	26.373	5.045	-124.487	-109.291	34.122
800	12.850	35.290	27.384	6.325	-124.412	-107.126	29.265
900	12.980	36.810	28.347	7.617	-124.377	-104.966	25.489
1000	13.150	38.190	29.267	8.923	-124.390	-102.812	22.469
1090	13.330	39.328	30.049	10.115	-124.450	-100.866	20.224
1090	13.330	39.328	30.049	10.115	-126.652	-100.866	20.224
1100	13.350	39.450	30.134	10.248	-126.654	-100.630	19.993
1200	13.600	40.620	30.957	11.595	-126.669	-98.260	17.895
1300	13.880	41.720	31.745	12.968	-126.662	-95.894	16.121
1400	14.210	42.760	32.494	14.372	-126.627	-93.527	14.600
1500	14.570	43.750	33.209	15.811	-126.562	-91.161	13.282
1600	14.980	44.710	33.905	17.288	-126.461	-88.815	12.131
1700*	15.430	45.630	34.566	18.809	-126.321	-86.463	11.115
1800	15.930	46.530	35.209	20.377	-126.136	-84.133	10.215
1800	15.930	46.530	35.209	20.377	-160.721	-84.133	10.215
1900	16.470	47.400	35.823	21.996	-160.080	-79.882	9.188
2000	17.050	48.260	36.424	23.672	-159.390	-75.679	8.270

*Data extrapolated above 1600 K.

Phase changes: 1090 K, melting point of Eu; $\Delta H^\circ = 2.202$ kcal/mol.
1800 K, boiling point of Eu; $\Delta H^\circ = 34.585$ kcal/mol.

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

298.15-2000 K: $C_p^\circ = 11.173 + 2.236 \times 10^{-3}T + 0.267 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 11.173 \times 10^{-3}T + 1.118 \times 10^{-6}T^2 - 0.267 \times 10^{-2}T^{-1} - 3.341$

Reaction equations (kcal/mol):

298.15-1090 K: $\Delta H_r^\circ = -125.824 + 2.706 \times 10^{-3}T - 1.322 \times 10^{-6}T^2 + 23.750T^{-1}$
 $\Delta G_r^\circ = -125.824 - 2.706 \times 10^{-3}T \ln T + 1.322 \times 10^{-6}T^2 + 11.875T^{-1} + 40.419 \times 10^{-9}T$
1090-1800 K: $\Delta H_r^\circ = -125.410 - 2.108 \times 10^{-3}T + 0.958 \times 10^{-6}T^2 - 60.850T^{-1}$
 $\Delta G_r^\circ = -125.410 + 2.108 \times 10^{-3}T \ln T - 0.958 \times 10^{-6}T^2 - 30.425T^{-1} + 8.891 \times 10^{-9}T$
1800-2000 K: $\Delta H_r^\circ = -168.223 + 2.922 \times 10^{-3}T + 0.703 \times 10^{-6}T^2 - 60.850T^{-1}$
 $\Delta G_r^\circ = -168.223 - 2.922 \times 10^{-3}T \ln T - 0.703 \times 10^{-6}T^2 - 30.425T^{-1} + 69.919 \times 10^{-9}T$

Sources: Enthalpy of formation based on Smoes (108) and Kaldis (60). Low-temperature heat capacities and entropy at 298 K based on Teaney (115). High-temperature data based on McMasters (78). Data extrapolated above 1600 K.

EuS(g)
Europium Monosulfide (ideal gas)
[Formation: $\text{Eu(c)} + \text{S(c,l)} = \text{EuS(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	8.400	65.000	65.000	0	24.000	12.450	-9.126
300	8.410	65.050	65.000	.016	23.994	12.380	-9.019
368.3	8.560	66.800	65.181	.597	23.737	9.761	-5.792
368.3	8.560	66.800	65.181	.597	23.641	9.761	-5.792
388.36	8.604	67.256	65.276	.769	23.560	9.008	-5.069
388.36	8.604	67.256	65.276	.769	23.147	9.008	-5.069
400	8.630	67.510	65.338	.869	23.082	8.585	-4.691
432.02	8.665	68.176	65.524	1.146	22.881	7.432	-3.760
500	8.740	69.440	65.964	1.738	22.334	5.052	-2.208
600	8.790	71.040	66.682	2.615	21.646	1.661	-.605
700	8.830	72.400	67.406	3.496	20.989	-1.619	.505
717.824	8.834	72.622	67.532	3.653	20.875	-2.192	.668

*Data except enthalpy of formation at 298 K estimated.

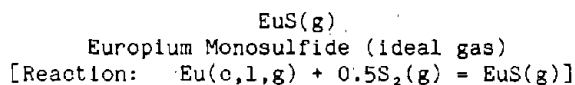
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $\text{Cp}^\circ = 8.910 + 0.018 \times 10^{-3}T - 0.457 \times 10^{-5}T^{-2}$
 $\text{H}^\circ - \text{H}^\circ_{298} = 8.910 \times 10^{-3}T + 0.009 \times 10^{-6}T^2 + 0.457 \times 10^{-2}T^{-1} - 2.811$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta \text{Hf}^\circ = 25.196 - 3.560 \times 10^{-3}T - 0.554 \times 10^{-6}T^2 - 25.300T^{-1}$
 $\Delta \text{Gf}^\circ = 25.196 + 3.560 \times 10^{-3}T \ln T + 0.554 \times 10^{-6}T^2 - 12.650T^{-1} - 63.055 \times 10^{-3}T$
368.3-388.36 K: $\Delta \text{Hf}^\circ = 24.080 - 1.297 \times 10^{-3}T - 2.300 \times 10^{-6}T^2 + 130.300T^{-1}$
 $\Delta \text{Gf}^\circ = 24.080 + 1.297 \times 10^{-3}T \ln T + 2.300 \times 10^{-6}T^2 + 65.150T^{-1} - 47.872 \times 10^{-3}T$
388.36-432.02 K: $\Delta \text{Hf}^\circ = 7.922 + 43.443 \times 10^{-3}T - 45.582 \times 10^{-6}T^2 + 2032.500T^{-1}$
 $\Delta \text{Gf}^\circ = 7.922 - 43.443 \times 10^{-3}T \ln T + 45.582 \times 10^{-6}T^2 + 1016.250T^{-1} + 237.356 \times 10^{-3}T$
432.02-717.824 K: $\Delta \text{Hf}^\circ = -1.557 + 39.537 \times 10^{-3}T - 25.770 \times 10^{-6}T^2 + 5259.000T^{-1}$
 $\Delta \text{Gf}^\circ = -1.557 - 39.537 \times 10^{-3}T \ln T + 25.770 \times 10^{-6}T^2 + 2629.500T^{-1} + 235.509 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15*	8.400	65.000	65.000	0	8.645	2.936	-2.152
300	8.410	65.050	65.000	.016	8.642	2.903	-2.114
400	8.630	67.510	65.338	.869	8.431	1.020	-.557
500	8.740	69.440	65.964	1.738	8.207	-.802	-.350
600	8.790	71.040	66.682	2.615	7.951	-2.580	.940
700	8.830	72.400	67.406	3.496	7.664	-4.314	1.347
800	8.850	73.580	68.104	4.381	7.344	-6.002	1.640
900	8.870	74.630	68.778	5.267	6.974	-7.654	1.859
1000	8.880	75.560	69.406	6.154	6.541	-9.251	2.022
1090	8.889	76.329	69.949	6.954	6.090	-10.657	2.137
1090	8.889	76.329	69.949	6.954	3.888	-10.657	2.137
1100	8.890	76.410	70.007	7.043	3.841	-10.791	2.144
1200	8.900	77.180	70.570	7.932	3.368	-12.095	2.203
1300	8.900	77.890	71.103	8.823	2.893	-13.360	2.246
1400	8.910	78.550	71.612	9.713	2.413	-14.592	2.278
1500	8.920	79.170	72.100	10.605	1.932	-15.797	2.302
1600	8.920	79.740	72.554	11.497	1.448	-16.954	2.316
1700	8.920	80.290	73.002	12.389	.959	-18.105	2.328
1800	8.930	80.800	73.422	13.281	.469	-19.215	2.333
1800	8.930	80.800	73.422	13.281	-34.116	-19.215	2.333
1900	8.930	81.280	73.820	14.174	-34.202	-18.376	2.114
2000	8.930	81.740	74.206	15.067	-34.295	-17.544	1.917

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1090 K, melting point of Eu; ΔH° = 2.202 kcal/mol.
1800 K, boiling point of Eu; ΔH° = 34.585 kcal/mol.

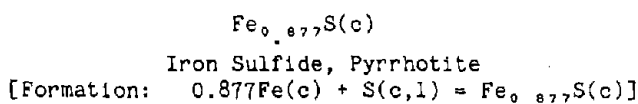
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $\text{Cp}^\circ = 8.910 + 0.018 \times 10^{-3}T - 0.457 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 8.910 \times 10^{-3}T + 0.009 \times 10^{-6}T^2 + 0.457 \times 10^{-2}T^{-1} - 2.811$

Reaction equations (kcal/mol):

298.15-1090 K: $\Delta\text{Hr}^\circ = 8.407 + 0.442 \times 10^{-3}T - 2.431 \times 10^{-6}T^2 + 96.150T^{-1}$
 $\Delta\text{Gr}^\circ = 8.407 - 0.442 \times 10^{-3}T \ln T + 2.431 \times 10^{-6}T^2 + 48.075T^{-1} - 17.092 \times 10^{-3}T$
1090-1800 K: $\Delta\text{Hr}^\circ = 8.821 - 4.372 \times 10^{-3}T - 0.151 \times 10^{-6}T^2 + 11.550T^{-1}$
 $\Delta\text{Gr}^\circ = 8.821 + 4.372 \times 10^{-3}T \ln T + 0.151 \times 10^{-6}T^2 + 5.775T^{-1} - 48.620 \times 10^{-3}T$
1800-2000 K: $\Delta\text{Hr}^\circ = -33.992 + 0.658 \times 10^{-3}T - 0.406 \times 10^{-6}T^2 + 11.550T^{-1}$
 $\Delta\text{Gr}^\circ = -33.992 - 0.658 \times 10^{-3}T \ln T + 0.406 \times 10^{-6}T^2 + 5.775T^{-1} + 12.409 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Smoes (108). Other data are those estimated by Mills (80).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	11.922	14.531	14.531	0	-25.200	-25.543	18.724
300	11.950	14.605	14.532	.022	-25.198	-25.546	18.610
368.3*	12.954	17.155	14.785	.873	-25.100	-25.634	15.211
368.3	12.954	17.155	14.785	.873	-25.196	-25.634	15.211
388.36	13.249	17.850	14.926	1.136	-25.165	-25.658	14.439
388.36	13.249	17.850	14.926	1.136	-25.578	-25.658	14.439
400	13.420	18.244	15.016	1.291	-25.578	-25.661	14.020
432.02	13.897	19.296	15.295	1.728	-25.589	-25.668	12.985
500	14.910	21.399	15.985	2.707	-25.697	-25.668	11.220
598	16.350	24.194	17.104	4.240	-25.637	-25.664	9.379
598	13.910	24.353	17.104	4.335	-25.542	-25.664	9.379
600	13.890	24.400	17.128	4.363	-25.544	-25.665	9.348
700	13.280	26.493	18.322	5.720	-25.684	-25.675	8.016
717.824	13.207	26.826	18.529	5.956	-25.716	-25.674	7.817

*Data above 350 K estimated.

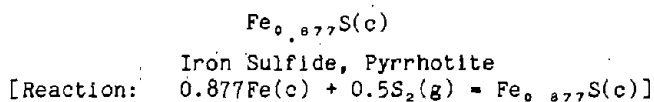
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 598 K, β - γ transition point of Fe_{0.877}S; ΔH° = 0.095 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-598 K: Cp° = 7.510 + 14.798x10⁻³T
 H° - H₂₉₈° = 7.510x10⁻³T + 7.399x10⁻⁶T² - 2.897
 598-1800 K: Cp° = -1.709 + 11.746x10⁻³T + 30.734x10⁻⁵T²
 H° - H₂₉₈° = -1.709x10⁻³T + 5.873x10⁻⁶T² - 30.734x10⁻²T⁻¹ + 8.396

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -25.547 - 0.470x10⁻³T + 3.792x10⁻⁶T² + 44.794T⁻¹
 ΔGf° = -25.547 + 0.470x10⁻³T lnT - 3.792x10⁻⁶T² + 22.397T⁻¹ - 1.788x10⁻³T
 368.3-388.36 K: ΔHf° = -26.662 + 1.793x10⁻³T + 2.046x10⁻⁶T² + 200.395T⁻¹
 ΔGf° = -26.662 - 1.793x10⁻³T lnT - 2.046x10⁻⁶T² + 100.197T⁻¹ + 13.395x10⁻³T
 388.36-432.02 K: ΔHf° = -42.821 + 46.533x10⁻³T - 41.236x10⁻⁶T² + 2102.594T⁻¹
 ΔGf° = -42.821 - 46.533x10⁻³T lnT + 41.236x10⁻⁶T² + 1051.297T⁻¹ + 298.623x10⁻³T
 432.02-598 K: ΔHf° = -52.299 + 42.627x10⁻³T - 21.424x10⁻⁶T² + 5329.095T⁻¹
 ΔGf° = -52.299 - 42.627x10⁻³T lnT + 21.424x10⁻⁶T² + 2664.547T⁻¹ + 296.776x10⁻³T
 598-717.824 K: ΔHf° = -41.006 + 33.408x10⁻³T - 22.950x10⁻⁶T² + 2255.695T⁻¹
 ΔGf° = -41.006 - 33.408x10⁻³T lnT + 22.950x10⁻⁶T² + 1127.847T⁻¹ + 222.333x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	11.922	14.531	14.531	0	-40.555	-35.057	25.697
300	11.950	14.605	14.532	.022	-40.550	-35.023	25.514
400*	13.420	18.244	15.016	1.291	-40.229	-33.227	18.154
500	14.910	21.399	15.985	2.707	-39.824	-31.522	13.778
598	16.350	24.194	17.104	4.240	-39.340	-29.937	10.941
598	13.910	24.353	17.104	4.335	-39.245	-29.937	10.941
600	13.890	24.400	17.128	4.363	-39.239	-29.906	10.893
700	13.280	26.493	18.322	5.720	-39.009	-28.370	8.857
800	12.870	28.238	19.456	7.026	-38.897	-26.859	7.338
900	12.640	29.740	20.517	8.301	-38.906	-25.356	6.157
1000	12.430	31.052	21.506	9.546	-39.101	-23.843	5.211
1043	12.778	31.583	21.911	10.088	-39.307	-23.183	4.858
1100	13.240	32.274	22.429	10.829	-39.434	-22.296	4.430
1185	13.997	33.288	23.172	11.987	-39.434	-20.972	3.868
1185	13.997	33.288	23.172	11.987	-39.622	-20.972	3.868
1200	14.130	33.465	23.300	12.198	-39.586	-20.737	3.777
1300	14.980	34.628	24.127	13.651	-39.307	-19.177	3.224
1400	16.060	35.776	24.917	15.202	-38.952	-17.640	2.754
1500	17.370	36.927	25.680	16.871	-38.500	-16.133	2.351
1600	18.920	38.097	26.419	18.685	-37.924	-14.659	2.002
1667	20.032	38.894	26.904	19.987	-37.465	-13.695	1.795
1667	20.032	38.894	26.904	19.987	-37.640	-13.695	1.795
1700	20.580	39.292	27.141	20.657	-37.410	-13.223	1.700
1800	22.590	40.524	27.851	22.812	-36.604	-11.823	1.436

*Data above 350 K estimated.

Phase changes: 598 K, β - γ transition point of Fe_{0.877}S; ΔH° = 0.095 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.

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

298.15-598 K: Cp° = 7.510 + 14.798x10⁻³T
H° - H₂₉₈° = 7.510x10⁻³T + 7.399x10⁻⁶T² - 2.897
598-1800 K: Cp° = -1.709 + 11.746x10⁻³T + 30.734x10⁻⁵T²
H° - H₂₉₈° = -1.709x10⁻³T + 5.873x10⁻⁵T² - 30.734x10⁻³T³ + 8.396

Reaction equations (kcal/mol):

298.15-598 K: ΔHr° = -42.336 + 3.532x10⁻³T + 1.915x10⁻⁶T² + 166.245T⁻¹
ΔGr° = -42.336 - 3.532x10⁻³TlnT - 1.915x10⁻⁶T² + 83.122T⁻¹ + 44.175x10⁻³T
598-1043 K: ΔHr° = -31.043 - 5.687x10⁻³T + 0.389x10⁻⁶T² - 2907.156T⁻¹
ΔGr° = -31.043 + 5.687x10⁻³TlnT - 0.389x10⁻⁶T² - 1453.578T⁻¹ - 30.268x10⁻³T
1043-1185 K: ΔHr° = -10.380 - 44.258x10⁻³T + 18.552x10⁻⁶T² - 3107.550T⁻¹
ΔGr° = -10.380 + 44.258x10⁻³TlnT - 18.552x10⁻⁶T² - 1553.775T⁻¹ - 299.107x10⁻³T
1185-1667 K: ΔHr° = -31.089 - 10.708x10⁻³T + 4.791x10⁻⁶T² - 3003.187T⁻¹
ΔGr° = -31.089 + 10.708x10⁻³TlnT - 4.791x10⁻⁶T² - 1501.594T⁻¹ - 60.527x10⁻³T
1667-1800 K: ΔHr° = -103.788 + 31.823x10⁻³T - 3.655x10⁻⁶T² + 38829.012T⁻¹
ΔGr° = -103.788 - 31.823x10⁻³TlnT + 3.655x10⁻⁶T² + 19414.506T⁻¹ + 277.011x10⁻³T

Source: Data from Chase (17) who estimated all above 350 K.

FeS(c)
Iron Monosulfide, Troilite
[Formation: Fe(c) + S(c,1) = FeS(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	12.080	14.415	14.415	0	-23.810	-23.880	17.504
300	12.110	14.490	14.417	.022	-23.809	-23.880	17.397
350	13.752	16.455	14.566	.661	-23.755	-23.896	14.921
368.3	15.344	17.196	14.679	.927	-23.709	-23.904	14.185
368.3	15.344	17.196	14.679	.927	-23.805	-23.904	14.185
388.36	17.090	18.018	14.830	1.238	-23.742	-23.910	13.455
388.36	17.090	18.018	14.830	1.238	-24.155	-23.910	13.455
400	18.103	18.538	14.931	1.443	-24.114	-23.904	13.060
411	19.544	19.048	15.034	1.650	-24.074	-23.899	12.708
411	17.350	20.411	15.034	2.210	-23.514	-23.899	12.708
432.02	17.350	21.276	15.317	2.575	-23.458	-23.921	12.101
500	17.350	23.812	16.304	3.754	-23.422	-23.993	10.487
598	17.350	26.917	17.795	5.455	-23.283	-24.116	8.813
598	14.642	27.076	17.795	5.550	-23.188	-24.116	8.813
600	14.633	27.125	17.827	5.579	-23.191	-24.119	8.785
700	14.265	29.351	19.318	7.023	-23.342	-24.262	7.575
717.824	14.230	29.709	19.572	7.277	-23.374	-24.284	7.394

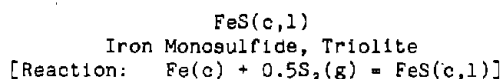
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 411 K, α - β transition point of FeS; ΔH° = 0.560 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 598 K, β - γ transition point of FeS; ΔH° = 0.095 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-411 K: Cp° = -80.385 + 199.956x10⁻³T + 29.540x10⁻⁵T²
 H° - H₂₉₈° = -80.385x10⁻³T + 99.978x10⁻⁶T² - 29.540x10⁻²T⁻¹ + 24.987
 411-598 K: Cp° = 17.351
 H° - H₂₉₈° = 17.351x10⁻³T - 4.921
 598-1465 K: Cp° = 6.041 + 6.678x10⁻³T + 16.479x10⁻⁵T²
 H° - H₂₉₈° = 6.041x10⁻³T + 3.339x10⁻⁶T² - 16.479x10⁻²T⁻¹ + 3.499

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 3.691 - 88.338x10⁻³T + 95.624x10⁻⁶T² - 2881.100T⁻¹
 ΔGf° = 3.691 + 88.338x10⁻³TlnT - 95.624x10⁻⁶T² - 1440.550T⁻¹ - 551.071x10⁻³T
 368.3-388.36 K: ΔHf° = 2.576 - 86.075x10⁻³T + 93.878x10⁻⁶T² - 2725.500T⁻¹
 ΔGf° = 2.576 + 86.075x10⁻³TlnT - 93.878x10⁻⁶T² - 1362.750T⁻¹ - 535.888x10⁻³T
 388.36-411 K: ΔHf° = -13.583 - 41.335x10⁻³T + 50.596x10⁻⁶T² - 823.300T⁻¹
 ΔGf° = -13.583 + 41.335x10⁻³TlnT - 50.596x10⁻⁶T² - 411.650T⁻¹ - 250.660x10⁻³T
 411-432.02 K: ΔHf° = -43.491 + 56.401x10⁻³T - 49.382x10⁻⁶T² + 2130.700T⁻¹
 ΔGf° = -43.491 - 56.401x10⁻³TlnT + 49.382x10⁻⁶T² + 1065.350T⁻¹ + 360.509x10⁻³T
 432.02-598 K: ΔHf° = -52.970 + 52.495x10⁻³T - 29.570x10⁻⁶T² + 5357.200T⁻¹
 ΔGf° = -52.970 - 52.495x10⁻³TlnT + 29.570x10⁻⁶T² + 2678.600T⁻¹ + 358.661x10⁻³T
 598-717.824 K: ΔHf° = -44.550 + 41.185x10⁻³T - 26.231x10⁻⁶T² + 3709.300T⁻¹
 ΔGf° = -44.550 - 41.185x10⁻³TlnT + 26.231x10⁻⁶T² + 1854.650T⁻¹ + 276.570x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	12.080	14.415	14.415	0	-39.165	-33.393	24.478
300	12.110	14.490	14.417	.022	-39.161	-33.358	24.301
350	13.752	16.455	14.566	.661	-39.026	-32.400	20.231
400	18.103	18.538	14.931	1.443	-38.765	-31.470	17.194
411	19.544	19.048	15.034	1.650	-38.675	-31.270	16.628
411	17.350	20.411	15.034	2.210	-38.115	-31.270	16.628
500	17.350	23.812	16.304	3.754	-37.549	-29.846	13.046
598	17.350	26.917	17.795	5.455	-36.986	-28.388	10.375
598	14.642	27.076	17.795	5.550	-36.891	-28.388	10.375
600	14.633	27.125	17.827	5.579	-36.885	-28.360	10.330
700	14.265	29.351	19.318	7.023	-36.667	-26.957	8.416
800	14.068	31.241	20.694	8.438	-36.553	-25.579	6.988
900	14.043	32.895	21.959	9.842	-36.550	-24.210	5.879
1000	14.190	34.381	23.129	11.252	-36.720	-22.833	4.990
1043	14.327	34.981	23.605	11.865	-36.933	-22.232	4.658
1100	14.509	35.747	24.214	12.686	-37.065	-21.422	4.256
1185	14.925	36.841	25.081	13.936	-37.083	-20.212	3.728
1185	14.925	36.841	25.081	13.936	-37.298	-20.212	3.728
1200	14.999	37.029	25.229	14.160	-37.264	-19.997	3.642
1300	15.661	38.255	26.185	15.691	-37.007	-18.569	3.122
1400	16.495	39.445	27.089	17.298	-36.700	-17.161	2.679
1465	17.130	40.208	27.655	18.390	-36.465	-16.260	2.426
1465	15.000	45.443	27.655	26.060	-28.795	-16.260	2.426
1500	15.000	45.797	28.074	26.585	-28.736	-15.961	2.325
1600	15.000	46.765	29.212	28.085	-28.582	-15.113	2.064

Phase changes: 411 K, α - β transition point of FeS; ΔH° = 0.560 kcal/mol.
598 K, β - γ transition point of FeS; ΔH° = 0.095 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.
1465 K, melting point of FeS; ΔH° = 7.670 kcal/mol.

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

298.15-411 K: Cp° = -80.385 + 199.956x10⁻³T + 29.540x10⁻⁵T²
H° - H₂₉₈° = -80.385x10⁻³T + 99.978x10⁻⁶T² - 29.540x10⁻²T³ + 24.987
411-598 K: Cp° = 17.351
H° - H₂₉₈° = 17.351x10⁻³T - 4.921
598-1465 K: Cp° = 6.041 + 6.678x10⁻³T + 16.479x10⁻⁵T²
H° - H₂₉₈° = 6.041x10⁻³T + 3.339x10⁻⁶T² - 16.479x10⁻²T³ + 3.499
1465-1600 K: Cp° = 15.000
H° - H₂₉₈° = 15.000x10⁻³T + 4.085

Reaction equations (kcal/mol):

298.15-411 K: ΔHr° = -13.098 - 84.335x10⁻³T + 93.747x10⁻⁶T² - 2759.650T⁻¹
ΔGr° = -13.098 + 84.335x10⁻³TlnT - 93.747x10⁻⁶T² - 1379.825T⁻¹ - 505.108x10⁻³T
411-598 K: ΔHr° = -43.006 + 13.400x10⁻³T - 6.231x10⁻⁶T² + 194.350T⁻¹
ΔGr° = -43.006 - 13.400x10⁻³TlnT + 6.231x10⁻⁶T² + 97.175T⁻¹ + 106.061x10⁻³T
598-1043 K: ΔHr° = -34.586 + 2.090x10⁻³T - 2.892x10⁻⁶T² - 1453.550T⁻¹
ΔGr° = -34.586 - 2.090x10⁻³TlnT + 2.892x10⁻⁶T² - 726.775T⁻¹ + 23.970x10⁻³T
1043-1185 K: ΔHr° = -11.026 - 41.891x10⁻³T + 17.819x10⁻⁶T² - 1682.050T⁻¹
ΔGr° = -11.026 + 41.891x10⁻³TlnT - 17.819x10⁻⁶T² - 841.025T⁻¹ - 282.575x10⁻³T
1185-1465 K: ΔHr° = -34.639 - 3.636x10⁻³T + 2.128x10⁻⁶T² - 1563.050T⁻¹
ΔGr° = -34.639 + 3.636x10⁻³TlnT - 2.128x10⁻⁶T² - 781.525T⁻¹ - 10.534x10⁻³T
1465-1600 K: ΔHr° = -34.053 + 5.323x10⁻³T - 1.211x10⁻⁶T² + 84.850T⁻¹
ΔGr° = -34.053 - 5.323x10⁻³TlnT + 1.211x10⁻⁶T² + 42.425T⁻¹ + 49.098x10⁻³T

Sources: Enthalpy of formation at 298 K from Adami (1). Low-temperature heat capacities and entropy at 298 K from Gronvold (48). High-temperature data based on Coughlin (25) and Vaisburd (122).

FeS(g)
Iron Monosulfide (ideal gas)
[Formation: Fe(c) + S(c,l) = FeS(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	9.277	60.785	60.785	0	88.615	74.720	-54.771
300	9.287	60.842	60.785	.017	88.611	74.634	-54.370
368.3	9.500	62.778	60.979	.662	88.451	71.468	-42.409
368.3	9.500	62.778	60.979	.662	88.355	71.468	-42.409
388.36	9.563	63.283	61.085	.853	88.298	70.551	-39.702
388.36	9.563	63.283	61.085	.853	87.885	70.551	-39.702
400	9.599	63.566	61.154	.965	87.833	70.032	-38.263
432.02	9.613	64.306	61.360	1.273	87.665	68.613	-34.709
500	9.644	65.716	61.860	1.928	87.177	65.654	-28.697
600	9.598	67.471	62.653	2.891	86.546	61.410	-22.368
700	9.530	68.945	63.449	3.847	85.907	57.271	-17.881
717.824	9.519	69.184	63.589	4.017	85.791	56.544	-17.215

*Data except enthalpy of formation at 298 K estimated.

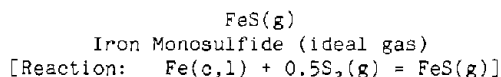
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2500 K: Cp° = 9.895 - 0.376x10⁻³T - 0.450x10⁻⁵T²
H° - H°₂₉₈ = 9.895x10⁻³T - 0.188x10⁻⁶T² + 0.450x10⁻²T³ - 3.084

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 88.044 + 1.942x10⁻³T - 4.542x10⁻⁶T² + 117.900T⁻¹
ΔGf° = 88.044 - 1.942x10⁻³TlnT + 4.542x10⁻⁶T² + 58.950T⁻¹ - 35.642x10⁻³T
368.3-388.36 K: ΔHf° = 86.929 + 4.205x10⁻³T - 6.288x10⁻⁶T² + 273.500T⁻¹
ΔGf° = 86.929 - 4.205x10⁻³TlnT + 6.288x10⁻⁶T² + 136.750T⁻¹ - 20.460x10⁻³T
388.36-432.02 K: ΔHf° = 70.771 + 48.945x10⁻³T - 49.570x10⁻⁶T² + 2175.700T⁻¹
ΔGf° = 70.771 - 48.945x10⁻³TlnT + 49.570x10⁻⁶T² + 1087.850T⁻¹ + 264.769x10⁻³T
432.02-717.824 K: ΔHf° = 61.292 + 45.039x10⁻³T - 29.758x10⁻⁶T² + 5402.200T⁻¹
ΔGf° = 61.292 - 45.039x10⁻³TlnT + 29.758x10⁻⁶T² + 2701.100T⁻¹ + 262.921x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15*	9.277	60.785	60.785	0	73.260	65.206	-47.797
300	9.287	60.842	60.785	.017	73.259	65.157	-47.466
400	9.599	63.566	61.154	.965	73.182	62.466	-34.130
500	9.644	65.716	61.860	1.928	73.049	59.801	-26.139
600	9.598	67.471	62.653	2.891	72.852	57.169	-20.824
700	9.530	68.945	63.449	3.847	72.582	54.576	-17.039
800	9.466	70.214	64.218	4.797	72.231	52.026	-14.213
900	9.411	71.325	64.946	5.741	71.773	49.527	-12.027
1000	9.366	72.314	65.635	6.679	71.132	47.086	-10.291
1043	9.351	72.708	65.919	7.081	70.709	46.061	-9.651
1100	9.331	73.205	66.283	7.614	70.287	44.727	-8.886
1185	9.308	73.899	66.805	8.406	69.813	42.769	-7.888
1185	9.308	73.899	66.805	8.406	69.598	42.769	-7.888
1200	9.304	74.016	66.894	8.546	69.547	42.429	-7.727
1300	9.283	74.760	67.472	9.475	69.202	40.183	-6.755
1400	9.267	75.447	68.016	10.403	68.830	37.966	-5.927
1500	9.255	76.086	68.533	11.329	68.434	35.775	-5.212
1600	9.247	76.683	69.024	12.254	68.012	33.612	-4.591
1667	9.243	77.063	69.341	12.873	67.715	32.175	-4.218
1667	9.243	77.063	69.341	12.873	67.515	32.175	-4.218
1700	9.241	77.244	69.492	13.178	67.340	31.477	-4.047
1800	9.238	77.772	69.938	14.102	66.791	29.385	-3.568
1811	9.238	77.828	69.985	14.204	66.726	29.153	-3.518
1811	9.238	77.828	69.985	14.204	63.426	29.153	-3.518
1900	9.236	78.271	70.363	15.026	62.846	27.484	-3.161
2000	9.236	78.745	70.770	15.950	62.191	25.639	-2.802
2100	9.238	79.196	71.161	16.873	61.534	23.825	-2.479
2200	9.241	79.625	71.535	17.797	60.874	22.047	-2.190
2300	9.245	80.036	71.896	18.721	60.212	20.297	-1.929
2400	9.250	80.430	72.244	19.646	59.549	18.574	-1.691
2500	9.257	80.808	72.579	20.572	58.886	16.881	-1.476

*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.

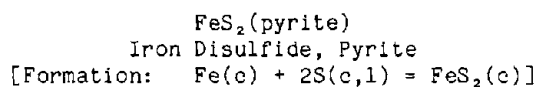
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $C_p^\circ = 9.895 - 0.376 \times 10^{-3}T + 0.450 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 9.895 \times 10^{-3}T - 0.188 \times 10^{-6}T^2 + 0.450 \times 10^{-2}T^3 - 3.084$

Reaction equations (kcal/mol):

298.15-1043 K: $\Delta H_r^\circ = 71.255 + 5.945 \times 10^{-3}T - 6.419 \times 10^{-6}T^2 + 239.350T^{-1}$
 $\Delta G_r^\circ = 71.255 - 5.945 \times 10^{-3}T \ln T + 6.419 \times 10^{-6}T^2 + 119.675T^{-1} + 10.320 \times 10^{-3}T$
1043-1185 K: $\Delta H_r^\circ = 94.816 - 38.036 \times 10^{-3}T + 14.292 \times 10^{-6}T^2 + 10.850T^{-1}$
 $\Delta G_r^\circ = 94.816 + 38.036 \times 10^{-3}T \ln T - 14.292 \times 10^{-6}T^2 + 5.425T^{-1} - 296.224 \times 10^{-3}T$
1185-1667 K: $\Delta H_r^\circ = 71.202 + 0.219 \times 10^{-3}T - 1.399 \times 10^{-6}T^2 + 129.850T^{-1}$
 $\Delta G_r^\circ = 71.202 - 0.219 \times 10^{-3}T \ln T + 1.399 \times 10^{-6}T^2 + 64.925T^{-1} - 24.183 \times 10^{-3}T$
1667-1811 K: $\Delta H_r^\circ = -11.692 + 48.716 \times 10^{-3}T - 11.030 \times 10^{-6}T^2 + 47829.050T^{-1}$
 $\Delta G_r^\circ = -11.692 - 48.716 \times 10^{-3}T \ln T + 11.030 \times 10^{-6}T^2 + 23914.525T^{-1} + 360.695 \times 10^{-3}T$
1811-2000 K: $\Delta H_r^\circ = 74.157 - 5.276 \times 10^{-3}T - 0.348 \times 10^{-6}T^2 + 10.850T^{-1}$
 $\Delta G_r^\circ = 74.157 + 5.276 \times 10^{-3}T \ln T + 0.348 \times 10^{-6}T^2 + 5.425T^{-1} - 65.103 \times 10^{-3}T$
2000-2500 K: $\Delta H_r^\circ = 75.182 - 5.860 \times 10^{-3}T - 0.238 \times 10^{-6}T^2 - 585.000T^{-1}$
 $\Delta G_r^\circ = 75.182 + 5.860 \times 10^{-3}T \ln T + 0.238 \times 10^{-6}T^2 - 292.500T^{-1} - 69.756 \times 10^{-3}T$

Source: Data from Chase (17) who estimated all except enthalpy of formation at 298 K.



T, K	cal/mol·K			kcal/mol			Log Kf.
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	14.848	12.647	12.647	0	-41.000	-38.259	28.044
300	14.887	12.739	12.647	.028	-41.003	-38.241	27.858
368.3	15.958	15.921	12.966	1.088	-41.132	-37.599	22.311
368.3	15.958	15.921	12.966	1.088	-41.324	-37.599	22.311
388.36	16.272	16.776	13.141	1.412	-41.368	-37.394	21.043
388.36	16.272	16.776	13.141	1.412	-42.194	-37.394	21.043
400	16.455	17.259	13.254	1.602	-42.255	-37.250	20.352
432.02	16.699	18.536	13.599	2.133	-42.462	-36.842	18.638
500	17.218	21.021	14.441	3.290	-43.123	-35.900	15.692
600	17.760	24.210	15.810	5.040	-43.824	-34.386	12.525
700	18.238	26.984	17.214	6.839	-44.420	-32.766	10.230
717.824	18.325	27.444	17.462	7.165	-44.517	-32.467	9.885

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1000 K: $C_p^\circ = 16.461 + 3.346 \times 10^{-3}T - 2.320 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 16.461 \times 10^{-3}T + 1.673 \times 10^{-6}T^2 + 2.320 \times 10^{-2}T^{-1} - 5.835$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -41.515 + 0.334 \times 10^{-3}T - 0.964 \times 10^{-6}T^2 + 149.300T^{-1}$
 $\Delta G_f^\circ = -41.515 - 0.334 \times 10^{-3}T \ln T + 0.964 \times 10^{-6}T^2 + 74.650T^{-1} + 11.697 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = -43.745 + 4.860 \times 10^{-3}T - 4.456 \times 10^{-6}T^2 + 460.500T^{-1}$
 $\Delta G_f^\circ = -43.745 - 4.860 \times 10^{-3}T \ln T + 4.456 \times 10^{-6}T^2 + 230.250T^{-1} + 42.063 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = -76.061 + 94.340 \times 10^{-3}T - 91.020 \times 10^{-6}T^2 + 4264.900T^{-1}$
 $\Delta G_f^\circ = -76.061 - 94.340 \times 10^{-3}T \ln T + 91.020 \times 10^{-6}T^2 + 2132.450T^{-1} + 612.520 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = -95.019 + 86.528 \times 10^{-3}T - 51.396 \times 10^{-6}T^2 + 10717.900T^{-1}$
 $\Delta G_f^\circ = -95.019 - 86.528 \times 10^{-3}T \ln T + 51.396 \times 10^{-6}T^2 + 5358.950T^{-1} + 608.825 \times 10^{-3}T$

FeS₂(marcasite)
Iron Disulfide, Marcasite
[Reaction: Fe(c) + S₂(g) = FeS₂(c)]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	14.912	12.874	12.874	0	-70.710	-56.353	41.308
300	14.951	12.966	12.874	.028	-70.707	-56.263	40.987
400	16.532	17.506	13.484	1.609	-70.550	-51.473	28.123
500	17.315	21.290	14.678	3.306	-70.362	-46.725	20.423
600	17.822	24.492	16.054	5.063	-70.190	-42.014	15.303
700*	18.394	27.280	17.461	6.873	-70.036	-37.329	11.655
800	18.802	29.773	18.848	8.740	-69.905	-32.667	8.924
900	19.292	32.016	20.188	10.645	-69.842	-28.017	6.803
1000	19.781	34.073	21.474	12.599	-69.911	-23.367	5.107

*Marcasite metastable above 673 K. Data extrapolated above 700 K.

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

298.15-1000 K: $C_p^\circ = 16.255 + 3.792 \times 10^{-3}T - 2.199 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 16.255 \times 10^{-3}T + 1.896 \times 10^{-6}T^2 + 2.199 \times 10^{-2}T^{-1} - 5.753$

Reaction equations (kcal/mol):

298.15-1000 K: $\Delta H_r^\circ = -74.010 + 8.133 \times 10^{-3}T - 4.495 \times 10^{-6}T^2 + 380.100T^{-1}$
 $\Delta G_r^\circ = -74.010 - 8.133 \times 10^{-3}T \ln T + 4.495 \times 10^{-6}T^2 + 190.050T^{-1} + 102.081 \times 10^{-3}T$

Source: Data from Chase (17) who extrapolated above 700 K.

FeS₂(marcasite)
Iron Disulfide, Marcasite
[Formation: Fe(c) + 2S(c,l) = FeS₂(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	14.912	12.874	12.874	0	-40.000	-37.326	27.360
300	14.951	12.966	12.874	.028	-40.003	-37.309	27.179
368.3	16.031	16.162	13.194	1.093	-40.128	-36.684	21.768
368.3	16.031	16.162	13.194	1.093	-40.320	-36.684	21.768
388.36	16.348	17.020	13.370	1.418	-40.362	-36.483	20.531
388.36	16.348	17.020	13.370	1.418	-41.188	-36.483	20.531
400	16.532	17.506	13.484	1.609	-41.248	-36.342	19.856
432.02	16.783	18.789	13.830	2.142	-41.453	-35.942	18.182
500	17.315	21.290	14.678	3.306	-42.107	-35.019	15.306
600	17.822	24.492	16.054	5.063	-42.801	-33.532	12.214
700*	18.394	27.280	17.461	6.873	-43.386	-31.939	9.972
717.824	18.467	27.743	17.711	7.201	-43.480	-31.645	9.635

*Marcasite metastable above 673 K.

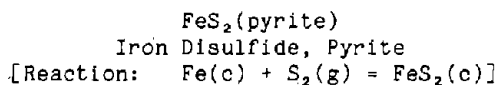
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1400 K: Cp° = 16.255 + 3.792x10⁻³T - 2.199x10⁻⁶T²
 H° - H°₂₉₈ = 16.255x10⁻³T + 1.896x10⁻⁶T² + 2.199x10⁻²T³ - 5.753

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -40.432 + 0.128x10⁻³T - 0.741x10⁻⁶T² + 137.200T⁻¹
 ΔGf° = -40.432 - 0.128x10⁻³TlnT + 0.741x10⁻⁶T² + 68.600T⁻¹ + 10.155x10⁻³T
 368.3-388.36 K: ΔHf° = -42.663 + 4.654x10⁻³T - 4.233x10⁻⁶T² + 448.400T⁻¹
 ΔGf° = -42.663 - 4.654x10⁻³TlnT + 4.233x10⁻⁶T² + 224.200T⁻¹ + 40.521x10⁻³T
 388.36-432.02 K: ΔHf° = -74.979 + 94.134x10⁻³T - 90.797x10⁻⁶T² + 4252.800T⁻¹
 ΔGf° = -74.979 - 94.134x10⁻³TlnT + 90.797x10⁻⁶T² + 2126.400T⁻¹ + 610.978x10⁻³T
 432.02-717.824 K: ΔHf° = -93.937 + 86.322x10⁻³T - 51.173x10⁻⁶T² + 10705.800T⁻¹
 ΔGf° = -93.937 - 86.322x10⁻³TlnT + 51.173x10⁻⁶T² + 5352.900T⁻¹ + 607.283x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	14.848	12.647	12.647	0	-71.710	-57.286	41.991
300	14.887	12.739	12.647	.028	-71.707	-57.195	41.666
400	16.455	17.259	13.254	1.602	-71.557	-52.381	28.619
500	17.218	21.021	14.441	3.290	-71.378	-47.606	20.809
600	17.760	24.210	15.810	5.040	-71.213	-42.868	15.614
700	18.238	26.984	17.214	6.839	-71.070	-38.156	11.913
800	18.727	29.451	18.591	8.688	-70.957	-33.461	9.141
900	19.217	31.685	19.924	10.585	-70.902	-28.779	6.988
1000	19.706	33.735	21.204	12.531	-70.979	-24.097	5.266

Phase change: 1016 K, incongruent melting point of FeS₂; decomposition pressure equals approximately 10 atm.

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

298.15-1000 K: $C_p^\circ = 16.461 + 3.346 \times 10^{-3}T - 2.320 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 16.461 \times 10^{-3}T + 1.673 \times 10^{-6}T^2 + 2.320 \times 10^{-2}T^{-1} - 5.835$

Reaction equations (kcal/mol):

298.15-1000 K: $\Delta H_r^\circ = -75.092 + 8.339 \times 10^{-3}T - 4.718 \times 10^{-5}T^2 + 392.200T^{-1}$
 $\Delta G_r^\circ = -75.092 - 8.339 \times 10^{-3}T \ln T + 4.718 \times 10^{-6}T^2 + 196.100T^{-1} + 103.623 \times 10^{-3}T$

Source: Data from Chase (17).

GaS(c)
Gallium Monosulfide
[Formation: Ga(c,l) + S(c,l) = GaS(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	11.020	13.820	13.820	0	-50.000	-48.927	35.864
300*	11.030	13.890	13.823	.020	-50.002	-48.921	35.639
302.9	11.056	13.996	13.824	.052	-50.005	-48.911	35.290
302.9	11.056	13.996	13.824	.052	-51.341	-48.911	35.290
368.3	11.652	16.216	14.055	.796	-51.398	-48.379	28.708
368.3	11.652	16.216	14.055	.796	-51.494	-48.379	28.708
388.36	11.834	16.839	14.183	1.032	-51.509	-48.209	27.129
388.36	11.834	16.839	14.183	1.032	-51.922	-48.209	27.129
400	11.940	17.190	14.265	1.170	-51.947	-48.097	26.279
432.02	12.199	18.119	14.517	1.556	-52.031	-47.787	24.174
500	12.750	19.940	15.120	2.410	-52.288	-47.088	20.582
600	13.450	22.330	16.130	3.720	-52.474	-46.029	16.766
700	14.050	24.450	17.179	5.090	-52.540	-44.955	14.035
717.824	14.137	24.804	17.364	5.341	-52.539	-44.761	13.628

*Data above 298 K estimated.

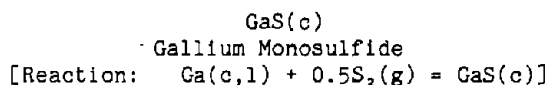
Phase changes: 302.9 K, melting point of Ga; ΔH° = 1.336 kcal/mol.
 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1000 K: Cp° = 10.705 + 4.912x10⁻³T - 1.021x10⁻⁵T⁻²
 H° - H°₂₉₈ = 10.705x10⁻³T + 2.456x10⁻⁶T² + 1.021x10⁻²T⁻¹ - 3.752

Formation equations (kcal/mol):

298.15-302.9 K: ΔHf° = -49.000 - 3.965x10⁻³T + 4.073x10⁻⁶T² - 53.500T⁻¹
 ΔGf° = -49.000 + 3.965x10⁻³T ln T - 4.073x10⁻⁶T² - 26.750T⁻¹ - 20.829x10⁻³T
 302.9-368.3 K: ΔHf° = -50.706 - 3.469x10⁻³T + 4.047x10⁻⁶T² + 13.700T⁻¹
 ΔGf° = -50.706 + 3.469x10⁻³T ln T - 4.047x10⁻⁶T² + 6.850T⁻¹ - 12.738x10⁻³T
 368.3-388.36 K: ΔHf° = -51.821 - 1.206x10⁻³T + 2.301x10⁻⁶T² + 169.300T⁻¹
 ΔGf° = -51.821 + 1.206x10⁻³T ln T - 2.301x10⁻⁶T² + 84.650T⁻¹ + 2.445x10⁻³T
 388.36-432.02 K: ΔHf° = -67.980 + 43.534x10⁻³T - 40.981x10⁻⁶T² + 2071.500T⁻¹
 ΔGf° = -67.980 - 43.534x10⁻³T ln T + 40.981x10⁻⁶T² + 1035.750T⁻¹ + 287.673x10⁻³T
 432.02-717.824 K: ΔHf° = -77.458 + 39.628x10⁻³T - 21.169x10⁻⁶T² + 5298.000T⁻¹
 ΔGf° = -77.458 - 39.628x10⁻³T ln T + 21.169x10⁻⁶T² + 2649.000T⁻¹ + 285.826x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	11.020	13.820	13.820	0	-65.355	-58.441	42.838
300*	11.030	13.890	13.823	.020	-65.354	-58.399	42.543
302.9	11.056	13.996	13.824	.052	-65.352	-58.332	42.087
302.9	11.056	13.996	13.824	.052	-66.688	-58.332	42.087
400	11.940	17.190	14.265	1.170	-66.598	-55.663	30.412
500	12.750	19.940	15.120	2.410	-66.416	-52.941	23.140
600	13.450	22.330	16.130	3.720	-66.169	-50.270	18.311
700	14.050	24.450	17.179	5.090	-65.865	-47.650	14.877
800	14.540	26.360	18.210	6.520	-65.506	-45.072	12.313
900	14.940	28.100	19.211	8.000	-65.101	-42.540	10.330
1000	15.230	29.690	20.180	9.510	-64.669	-40.055	8.754

*Data above 298 K estimated.

Phase change: 302.9 K, melting point of Ga; $\Delta H^\circ = 1.336$ kcal/mol.

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

298.15-1000 K: $\text{Cp}^\circ = 10.705 + 4.912 \times 10^{-3}T - 1.021 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 10.705 \times 10^{-3}T + 2.456 \times 10^{-6}T^2 + 1.021 \times 10^{-2}T^{-1} - 3.752$

Reaction equations (kcal/mol):

298.15-302.9 K: $\Delta \text{Hr}^\circ = -65.789 + 0.037 \times 10^{-3}T + 2.196 \times 10^{-6}T^2 + 67.950T^{-1}$
 $\Delta \text{Gr}^\circ = -65.789 - 0.037 \times 10^{-3}T \ln T - 2.196 \times 10^{-6}T^2 + 33.975T^{-1} + 25.134 \times 10^{-3}T$
302.9-1000 K: $\Delta \text{Hr}^\circ = -67.495 + 0.533 \times 10^{-3}T + 2.170 \times 10^{-6}T^2 + 135.150T^{-1}$
 $\Delta \text{Gr}^\circ = -67.495 - 0.533 \times 10^{-3}T \ln T - 2.170 \times 10^{-6}T^2 + 67.575T^{-1} + 33.225 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mills (80). Low-temperature heat capacities and entropy at 298 K from Mamedov (76). Data above 298 K estimated.

GdS(c)
Gadolinium Monosulfide
[Formation: $\text{Gd(c)} + \text{S(c,l)} = \text{GdS(c)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	11.500	20.330	20.330	0	-109.200	-108.135	79.264
300*	11.510	20.400	20.330	.021	-109.205	-108.129	78.771
368.3	11.804	22.800	20.574	.820	-109.303	-107.877	64.014
368.3	11.804	22.800	20.574	.820	-109.399	-107.877	64.014
388.36	11.890	23.428	20.706	1.057	-109.425	-107.793	60.660
388.36	11.890	23.428	20.706	1.057	-109.838	-107.793	60.660
400	11.940	23.780	20.790	1.196	-109.867	-107.731	58.861
432.02	12.017	24.702	21.046	1.580	-109.962	-107.557	54.410
500	12.180	26.470	21.664	2.403	-110.270	-107.151	46.835
600	12.350	28.710	22.660	3.630	-110.586	-106.487	38.787
700	12.490	30.620	23.659	4.873	-110.849	-105.777	33.025
717.824	12.513	30.934	23.835	5.096	-110.891	-105.647	32.165

*Data above 298 K estimated.

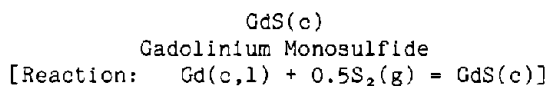
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: $C_p^\circ = 12.003 + 0.902 \times 10^{-3}T - 0.682 \times 10^{-5}T^2$
 $H^\circ - H^\circ_{298} = 12.003 \times 10^{-3}T + 0.451 \times 10^{-6}T^2 + 0.682 \times 10^{-2}T^{-1} - 3.848$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -110.634 + 1.043 \times 10^{-3}T - 0.035 \times 10^{-6}T^2 + 335.700T^{-1}$
 $\Delta G_f^\circ = -110.634 - 1.043 \times 10^{-3}T \ln T + 0.035 \times 10^{-6}T^2 + 167.850T^{-1} + 12.424 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -111.749 + 3.306 \times 10^{-3}T - 1.781 \times 10^{-6}T^2 + 491.300T^{-1}$
 $\Delta G_f^\circ = -111.749 - 3.306 \times 10^{-3}T \ln T + 1.781 \times 10^{-6}T^2 + 245.650T^{-1} + 27.607 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -127.907 + 48.046 \times 10^{-3}T - 45.063 \times 10^{-6}T^2 + 2393.500T^{-1}$
 $\Delta G_f^\circ = -127.907 - 48.046 \times 10^{-3}T \ln T + 45.063 \times 10^{-6}T^2 + 1196.750T^{-1} + 312.835 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -137.386 + 44.140 \times 10^{-3}T - 25.251 \times 10^{-6}T^2 + 5620.000T^{-1}$
 $\Delta G_f^\circ = -137.386 - 44.140 \times 10^{-3}T \ln T + 25.251 \times 10^{-6}T^2 + 2810.000T^{-1} + 310.988 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	11.500	20.330	20.330	0	-124.555	-117.649	86.238
300*	11.510	20.400	20.330	.021	-124.557	-117.607	85.675
400	11.940	23.780	20.790	1.196	-124.518	-115.297	62.995
500	12.180	26.470	21.664	2.403	-124.397	-113.005	49.394
600	12.350	28.710	22.660	3.630	-124.281	-110.728	40.332
700	12.490	30.620	23.659	4.873	-124.174	-108.472	33.866
800	12.620	32.300	24.639	6.129	-124.080	-106.238	29.022
900	12.730	33.790	25.572	7.396	-124.001	-104.011	25.257
1000	12.840	35.140	26.466	8.674	-123.933	-101.804	22.249
1100	12.940	36.370	27.313	9.963	-123.879	-99.585	19.785
1200	13.040	37.500	28.115	11.262	-123.842	-97.385	17.736
1300	13.130	38.540	28.871	12.570	-123.827	-95.174	16.000
1400	13.230	39.520	29.599	13.889	-123.833	-92.962	14.512
1500	13.320	40.440	30.296	15.216	-123.866	-90.761	13.224
1533	13.353	40.730	30.517	15.656	-123.884	-90.034	12.835
1533	13.353	40.730	30.517	15.656	-124.819	-90.034	12.835
1585	13.405	41.174	30.856	16.353	-124.719	-88.860	12.252
1585	13.405	41.174	30.856	16.353	-127.122	-88.860	12.252
1600	13.420	41.300	30.954	16.554	-127.124	-88.500	12.088
1700	13.510	42.120	31.591	17.900	-127.135	-86.090	11.067
1800	13.600	42.890	32.192	19.256	-127.140	-83.661	10.158
1900	13.700	43.630	32.777	20.621	-127.138	-81.250	9.346
2000	13.790	44.330	33.333	21.995	-127.131	-78.836	8.615

*Data above 298 K estimated.

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: $\text{Cp}^\circ = 12.003 + 0.902 \times 10^{-3}T - 0.682 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 12.003 \times 10^{-3}T + 0.451 \times 10^{-6}T^2 + 0.682 \times 10^{-2}T^{-1} - 3.848$

Reaction equations (kcal/mol):

298.15-1533 K: $\Delta\text{Hr}^\circ = -127.423 + 5.045 \times 10^{-3}T - 1.912 \times 10^{-6}T^2 + 457.150T^{-1}$
 $\Delta\text{Gr}^\circ = -127.423 - 5.045 \times 10^{-3}T \ln T + 1.912 \times 10^{-6}T^2 + 228.575T^{-1} + 58.387 \times 10^{-3}T$
1533-1585 K: $\Delta\text{Hr}^\circ = -127.064 + 1.004 \times 10^{-3}T + 0.291 \times 10^{-6}T^2 + 34.050T^{-1}$
 $\Delta\text{Gr}^\circ = -127.064 - 1.004 \times 10^{-3}T \ln T - 0.291 \times 10^{-6}T^2 + 17.025T^{-1} + 31.980 \times 10^{-3}T$
1585-2000 K: $\Delta\text{Hr}^\circ = -126.213 - 1.049 \times 10^{-3}T + 0.291 \times 10^{-6}T^2 + 34.050T^{-1}$
 $\Delta\text{Gr}^\circ = -126.213 + 1.049 \times 10^{-3}T \ln T - 0.291 \times 10^{-6}T^2 + 17.025T^{-1} + 16.315 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Fries (42). Low-temperature heat capacities and entropy at 298 K from Vasiliev (123). Data above 298 K estimated.

GdS(g)
Gadolinium Monosulfide (ideal gas)
[Formation: $\text{Gd(c)} + \text{S(c,l)} = \text{GdS(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	8.200	63.220	63.220	0	36.700	24.977	-18.308
300	8.210	63.270	63.220	.015	36.689	24.903	-18.142
368.3	8.415	64.981	63.394	.585	36.362	22.253	-13.205
368.3	8.415	64.981	63.394	.585	36.266	22.253	-13.205
388.36	8.475	65.429	63.487	.754	36.172	21.492	-12.095
388.36	8.475	65.429	63.487	.754	35.759	21.492	-12.095
400	8.510	65.680	63.548	.853	35.690	21.066	-11.510
432.02	8.555	66.337	63.730	1.126	35.485	19.902	-10.068
500	8.650	67.590	64.166	1.712	34.939	17.498	-7.648
600	8.730	69.180	64.878	2.581	34.265	14.082	-5.129
700	8.780	70.530	65.593	3.456	33.634	10.769	-3.362
717.824	8.785	70.751	65.718	3.613	33.525	10.189	-3.102

*Data except enthalpy of formation at 298 K estimated.

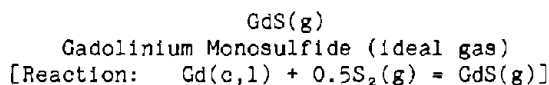
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: $C_p^\circ = 8.875 + 0.036 \times 10^{-3}T - 0.608 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 8.875 \times 10^{-3}T + 0.018 \times 10^{-6}T^2 + 0.608 \times 10^{-3}T^{-1} - 2.852$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 36.262 - 2.085 \times 10^{-3}T - 0.468 \times 10^{-6}T^2 + 328.300T^{-1}$
 $\Delta G_f^\circ = 36.262 + 2.085 \times 10^{-3}T \ln T + 0.468 \times 10^{-6}T^2 + 164.150T^{-1} - 51.716 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = 35.147 + 0.178 \times 10^{-3}T - 2.214 \times 10^{-6}T^2 + 483.900T^{-1}$
 $\Delta G_f^\circ = 35.147 - 0.178 \times 10^{-3}T \ln T + 2.214 \times 10^{-6}T^2 + 241.950T^{-1} - 36.533 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = 18.989 + 44.918 \times 10^{-3}T - 45.496 \times 10^{-6}T^2 + 2386.100T^{-1}$
 $\Delta G_f^\circ = 18.989 - 44.918 \times 10^{-3}T \ln T + 45.496 \times 10^{-6}T^2 + 1193.050T^{-1} + 248.695 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = 9.510 + 41.012 \times 10^{-3}T - 25.684 \times 10^{-6}T^2 + 5612.600T^{-1}$
 $\Delta G_f^\circ = 9.510 - 41.012 \times 10^{-3}T \ln T + 25.684 \times 10^{-6}T^2 + 2806.300T^{-1} + 246.848 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15*	8.200	63.220	63.220	0	21.345	15.463	-11.335
300	8.210	63.270	63.220	.015	21.337	15.426	-11.238
400	8.510	65.680	63.548	.853	21.039	13.500	-7.376
500	8.650	67.590	64.166	1.712	20.812	11.644	-5.090
600	8.730	69.180	64.878	2.581	20.571	9.841	-3.585
700	8.780	70.530	65.593	3.456	20.309	8.074	-2.521
800	8.810	71.700	66.281	4.335	20.025	6.348	-1.734
900	8.830	72.740	66.943	5.217	19.721	4.655	-1.130
1000	8.850	73.670	67.568	6.102	19.395	2.994	-.654
1100	8.860	74.520	68.168	6.987	19.045	1.374	-.273
1200	8.880	75.290	68.728	7.874	18.670	-.222	.040
1300	8.880	76.000	69.260	8.762	18.265	-1.780	.299
1400	8.890	76.660	69.766	9.651	17.829	-3.296	.515
1500	8.900	77.270	70.243	10.541	17.360	-4.781	.697
1533	8.903	77.464	70.396	10.835	17.195	-5.268	.751
1533	8.903	77.464	70.396	10.835	16.260	-5.268	.751
1585	8.908	77.766	70.638	11.298	16.126	-6.013	.829
1585	8.908	77.766	70.638	11.298	13.723	-6.013	.829
1600	8.910	77.850	70.705	11.432	13.654	-6.202	.847
1700	8.910	78.390	71.141	12.323	13.188	-7.426	.955
1800	8.920	78.900	71.559	13.214	12.719	-8.621	1.047
1900	8.930	79.380	71.955	14.107	12.248	-9.789	1.126
2000	8.930	79.840	72.340	15.000	11.774	-10.951	1.197

*Data except enthalpy of formation at 298 K estimated.

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: $C_p^\circ = 8.875 + 0.036 \times 10^{-3}T - 0.608 \times 10^{-5}T^2$
 $H^\circ - H^\circ_{298} = 8.875 \times 10^{-3}T + 0.018 \times 10^{-6}T^2 + 0.608 \times 10^{-2}T^{-1} - 2.852$

Reaction equations (kcal/mol):

298.15-1533 K: $\Delta H_r^\circ = 19.473 + 1.918 \times 10^{-3}T - 2.345 \times 10^{-6}T^2 + 449.750T^{-1}$
 $\Delta G_r^\circ = 19.473 - 1.918 \times 10^{-3}T \ln T + 2.345 \times 10^{-6}T^2 + 224.875T^{-1} - 5.753 \times 10^{-3}T$
1533-1585 K: $\Delta H_r^\circ = 19.832 - 2.124 \times 10^{-3}T - 0.142 \times 10^{-6}T^2 + 26.650T^{-1}$
 $\Delta G_r^\circ = 19.832 + 2.124 \times 10^{-3}T \ln T + 0.142 \times 10^{-6}T^2 + 13.325T^{-1} - 32.160 \times 10^{-3}T$
1585-2000 K: $\Delta H_r^\circ = 20.683 - 4.177 \times 10^{-3}T - 0.142 \times 10^{-6}T^2 + 26.650T^{-1}$
 $\Delta G_r^\circ = 20.683 + 4.177 \times 10^{-3}T \ln T + 0.142 \times 10^{-6}T^2 + 13.325T^{-1} - 47.824 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Fries (42). Other data are those estimated by Mills (80).

GeS(c)
Germanium Monosulfide
[Formation: Ge(c) + S(c,l) = GeS(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	11.420	15.770	15.770	0	-18.200	-18.402	13.489
300*	11.430	15.840	15.770	.021	-18.199	-18.405	13.407
368.3	11.758	18.223	16.010	.815	-18.180	-18.455	10.951
368.3	11.758	18.223	16.010	.815	-18.276	-18.455	10.951
388.36	11.854	18.849	16.141	1.052	-18.274	-18.464	10.391
388.36	11.854	18.849	16.141	1.052	-18.667	-18.464	10.391
400	11.910	19.200	16.225	1.190	-18.705	-18.457	10.085
432.02	12.067	20.123	16.480	1.574	-18.772	-18.436	9.326
500	12.400	21.910	17.100	2.405	-19.017	-18.358	8.024
600	12.880	24.210	18.095	3.669	-19.210	-18.201	6.630
700	13.360	26.230	19.116	4.980	-19.306	-18.028	5.628
717.824	13.446	26.567	19.297	5.219	-19.313	-17.995	5.479

*Data above 298 K estimated.

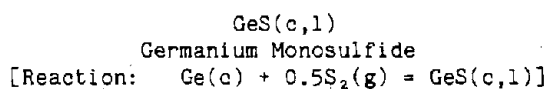
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-938 K: Cp° = 9.990 + 4.814x10⁻³T
H° - H°₂₉₈ = 9.990x10⁻³T + 2.407x10⁻⁶T² - 3.192

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -16.797 - 3.765x10⁻³T + 3.658x10⁻⁶T² - 180.500T⁻¹
ΔGf° = -16.797 + 3.765x10⁻³TlnT - 3.658x10⁻⁶T² - 90.250T⁻¹ - 24.729x10⁻³T
368.3-388.36 K: ΔHf° = -17.912 - 1.502x10⁻³T + 1.912x10⁻⁶T² - 24.900T⁻¹
ΔGf° = -17.912 + 1.502x10⁻³TlnT - 1.912x10⁻⁶T² - 12.450T⁻¹ - 9.546x10⁻³T
388.36-432.02 K: ΔHf° = -34.071 + 43.238x10⁻³T - 41.370x10⁻⁶T² + 1877.300T⁻¹
ΔGf° = -34.071 - 43.238x10⁻³TlnT + 41.370x10⁻⁶T² + 938.650T⁻¹ + 275.682x10⁻³T
432.02-717.824 K: ΔHf° = -43.549 + 39.332x10⁻³T - 21.558x10⁻⁶T² + 5103.800T⁻¹
ΔGf° = -43.549 - 39.332x10⁻³TlnT + 21.558x10⁻⁶T² + 2551.900T⁻¹ + 273.834x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	11.420	15.770	15.770	0	-33.555	-27.916	20.463
300*	11.430	15.840	15.770	.021	-33.551	-27.882	20.312
400	11.910	19.200	16.225	1.190	-33.356	-26.023	14.218
500	12.400	21.910	17.100	2.405	-33.145	-24.212	10.583
600	12.880	24.210	18.095	3.669	-32.904	-22.442	8.174
700	13.360	26.230	19.116	4.980	-32.631	-20.723	6.470
800	13.840	28.050	20.125	6.340	-32.321	-19.046	5.203
900	14.320	29.710	21.101	7.748	-31.979	-17.407	4.227
938	14.500	30.300	21.456	8.296	-31.840	-16.788	3.912
938	14.500	36.300	21.456	13.924	-26.212	-16.788	3.912
1000	14.500	37.230	22.407	14.823	-25.989	-16.181	3.536
1100	14.500	38.610	23.816	16.273	-25.646	-15.212	3.022

*Data above 298 K estimated except temperature and enthalpy of fusion.

Phase change: 938 K, melting point of GeS; $\Delta H^\circ = 5.628$ kcal/mol.

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

298.15-938 K: $C_p^\circ = 9.990 + 4.814 \times 10^{-3}T$
 $H^\circ - H_{298}^\circ = 9.990 \times 10^{-3}T + 2.407 \times 10^{-6}T^2 - 3.192$
 938-1100 K: $C_p^\circ = 14.500$
 $H^\circ - H_{298}^\circ = 14.500 \times 10^{-3}T + 0.323$

Reaction equations (kcal/mol):

298.15-938 K: $\Delta H_r^\circ = -33.586 + 0.238 \times 10^{-3}T + 1.781 \times 10^{-6}T^2 - 59.050T^{-1}$
 $\Delta G_r^\circ = -33.586 - 0.238 \times 10^{-3}T \ln T - 1.781 \times 10^{-6}T^2 - 29.525T^{-1} + 21.234 \times 10^{-3}T$
 938-1100 K: $\Delta H_r^\circ = -30.071 + 4.747 \times 10^{-3}T - 0.626 \times 10^{-6}T^2 - 59.050T^{-1}$
 $\Delta G_r^\circ = -30.071 - 4.747 \times 10^{-3}T \ln T + 0.626 \times 10^{-6}T^2 - 29.525T^{-1} + 46.093 \times 10^{-3}T$

Source: Data from Mills (80) who estimated all above 298 K except temperature and enthalpy of fusion.

GeS(g)
Germanium Monosulfide (ideal gas)
[Formation: $\text{Ge(c)} + \text{S(c,l)} = \text{GeS(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	8.040	56.260	56.260	0	23.200	10.925	-8.008
300	8.050	56.310	56.260	.015	23.195	10.848	-7.903
368.3	8.289	57.991	56.428	.575	22.981	8.059	-4.782
368.3	8.289	57.991	56.428	.575	22.885	8.059	-4.782
388.36	8.359	58.433	56.521	.742	22.816	7.254	-4.082
388.36	8.359	58.433	56.521	.742	22.403	7.254	-4.082
400	8.400	58.680	56.580	.840	22.345	6.801	-3.716
432.02	8.451	59.329	56.760	1.110	22.164	5.563	-2.814
500	8.560	60.580	57.202	1.689	21.667	2.990	-1.307
600	8.650	62.150	57.900	2.550	21.071	-.684	.249
700	8.710	63.480	58.597	3.418	20.532	-4.265	1.332
717.824	8.717	63.699	58.721	3.573	20.441	-4.894	1.490

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $C_p^\circ = 8.780 + 0.100 \times 10^{-3}T - 0.680 \times 10^{-5}T^2$
 $H^\circ - H^\circ_{298} = 8.780 \times 10^{-3}T + 0.050 \times 10^{-6}T^2 + 0.680 \times 10^{-2}T^{-1} - 2.850$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 24.945 - 4.975 \times 10^{-3}T + 1.301 \times 10^{-6}T^2 - 112.500T^{-1}$
 $\Delta G_f^\circ = 24.945 + 4.975 \times 10^{-3}T \ln T - 1.301 \times 10^{-6}T^2 - 56.250T^{-1} - 74.347 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = 23.830 - 2.712 \times 10^{-3}T - 0.445 \times 10^{-6}T^2 + 43.100T^{-1}$
 $\Delta G_f^\circ = 23.830 + 2.712 \times 10^{-3}T \ln T + 0.445 \times 10^{-6}T^2 + 21.550T^{-1} - 59.164 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = 7.672 + 42.028 \times 10^{-3}T - 43.727 \times 10^{-6}T^2 + 1945.300T^{-1}$
 $\Delta G_f^\circ = 7.672 - 42.028 \times 10^{-3}T \ln T + 43.727 \times 10^{-6}T^2 + 972.650T^{-1} + 226.065 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -1.807 + 38.122 \times 10^{-3}T - 23.915 \times 10^{-6}T^2 + 5171.800T^{-1}$
 $\Delta G_f^\circ = -1.807 - 38.122 \times 10^{-3}T \ln T + 23.915 \times 10^{-6}T^2 + 2585.900T^{-1} + 224.217 \times 10^{-3}T$

GeS(g)
Germanium Monosulfide (ideal gas)
[Reaction: $\text{Ge(c,l)} + 0.5\text{S}_2(\text{g}) = \text{GeS(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15	8.040	56.260	56.260	0	7.845	1.412	-1.035
300	8.050	56.310	56.260	.015	7.843	1.371	-.999
400	8.400	58.680	56.580	.840	7.694	-.765	-.418
500	8.560	60.580	57.202	1.689	7.540	-2.863	1.251
600	8.650	62.150	57.900	2.550	7.377	-4.925	1.794
700	8.710	63.480	58.597	3.418	7.207	-6.960	2.173
800	8.750	64.650	59.286	4.291	7.031	-8.975	2.452
900	8.790	65.680	59.938	5.168	6.842	-10.960	2.661
1000	8.810	66.610	60.562	6.048	6.636	-12.936	2.827
1100	8.830	67.450	61.149	6.931	6.413	-14.878	2.956
1200	8.850	68.220	61.708	7.815	6.170	-16.802	3.060
1210.4	8.852	68.296	61.764	7.907	6.143	-16.996	3.069
1210.4	8.852	68.296	61.764	7.907	-2.687	-16.996	3.069
1300	8.870	68.930	62.237	8.701	-2.890	-18.047	3.034
1400	8.890	69.590	62.741	9.589	-3.120	-19.205	2.998
1500	8.900	70.200	63.215	10.478	-3.354	-20.334	2.963
1600	8.910	70.780	63.674	11.369	-3.588	-21.476	2.933
1700	8.930	71.320	64.108	12.261	-3.825	-22.586	2.904
1800	8.940	71.830	64.522	13.154	-4.064	-23.676	2.875
1900	8.950	72.310	64.916	14.049	-4.305	-24.746	2.846
2000	8.960	72.770	65.298	14.944	-4.549	-25.814	2.821

Phase change: 1210.4 K, melting point of Ge; $\Delta H^\circ = 8.830$ kcal/mol.

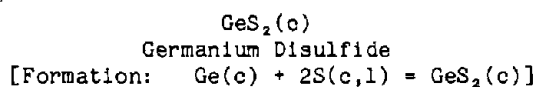
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 8.780 + 0.100 \times 10^{-3}T - 0.680 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 8.780 \times 10^{-3}T + 0.050 \times 10^{-6}T^2 + 0.680 \times 10^{-2}T^{-1} - 2.850$

Reaction equations (kcal/mol):

298.15-1210.4 K: $\Delta H_r^\circ = 8.156 - 0.973 \times 10^{-3}T - 0.576 \times 10^{-6}T^2 + 8.950T^{-1}$
 $\Delta G_r^\circ = 8.156 + 0.973 \times 10^{-3}T \ln T + 0.576 \times 10^{-6}T^2 + 4.475T^{-1} - 28.384 \times 10^{-3}T$
1210.4-2000 K: $\Delta H_r^\circ = -0.144 - 1.992 \times 10^{-3}T - 0.110 \times 10^{-6}T^2 + 33.850T^{-1}$
 $\Delta G_r^\circ = -0.144 + 1.992 \times 10^{-3}T \ln T + 0.110 \times 10^{-6}T^2 + 16.925T^{-1} - 28.204 \times 10^{-3}T$

Source: Data from Mills (80).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	15.700	22.370	22.370	0	-29.800	-29.686	21.760
300*	15.714	22.467	22.370	.029	-29.801	-29.686	21.626
368.3	16.116	25.738	22.702	1.118	-29.871	-29.655	17.597
368.3	16.116	25.738	22.702	1.118	-30.063	-29.655	17.597
388.36	16.234	26.596	22.881	1.443	-30.092	-29.631	16.675
388.36	16.234	26.596	22.881	1.443	-30.918	-29.631	16.675
400	16.303	27.076	22.996	1.632	-30.973	-29.592	16.168
432.02	16.435	28.337	23.346	2.156	-31.163	-29.476	14.911
500	16.714	30.760	24.192	3.284	-31.785	-29.153	12.743
600	17.056	33.838	25.550	4.973	-32.410	-28.560	10.403
700	17.366	36.491	26.928	6.694	-32.896	-27.883	8.705
717.824	17.418	36.928	27.171	7.004	-32.969	-27.754	8.450

*Data above 298 K estimated except temperature and enthalpy of fusion.

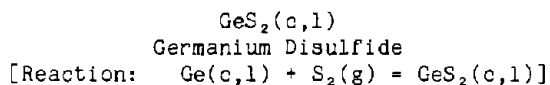
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1113 K: Cp° = 15.665 + 2.624x10⁻³T - 0.664x10⁻⁵T²
H° - H°₂₉₈ = 15.665x10⁻³T + 1.312x10⁻⁵T² + 0.664x10⁻²T⁻¹ - 5.010

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -27.408 - 6.264x10⁻³T + 4.280x10⁻⁶T² - 269.700T⁻¹
ΔGf° = -27.408 + 6.264x10⁻³TlnT - 4.280x10⁻⁶T² - 134.850T⁻¹ - 40.537x10⁻³T
368.3-388.36 K: ΔHf° = -29.638 - 1.738x10⁻³T + 0.788x10⁻⁶T² + 41.500T⁻¹
ΔGf° = -29.638 + 1.738x10⁻³TlnT - 0.788x10⁻⁶T² + 20.750T⁻¹ - 10.171x10⁻³T
388.36-432.02 K: ΔHf° = -61.955 + 87.742x10⁻³T - 85.776x10⁻⁶T² + 3845.900T⁻¹
ΔGf° = -61.955 - 87.742x10⁻³TlnT + 85.776x10⁻⁶T² + 1922.950T⁻¹ + 560.286x10⁻³T
432.02-717.824 K: ΔHf° = -80.912 + 79.930x10⁻³T - 46.152x10⁻⁶T² + 10298.900T⁻¹
ΔGf° = -80.912 - 79.930x10⁻³TlnT + 46.152x10⁻⁶T² + 5149.450T⁻¹ + 556.591x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	15.700	22.370	22.370	0	-60.510	-48.713	35.707
300*	15.714	22.467	22.370	.029	-60.505	-48.641	35.434
400	16.303	27.076	22.996	1.632	-60.275	-44.723	24.435
500	16.714	30.760	24.192	3.284	-60.040	-40.859	17.859
600	17.056	33.838	25.550	4.973	-59.799	-37.042	13.492
700	17.366	36.491	26.928	6.694	-59.546	-33.274	10.388
800	17.658	38.829	28.271	8.446	-59.279	-29.537	8.069
900	17.941	40.926	29.565	10.225	-59.006	-25.836	6.274
1000	18.217	42.830	30.797	12.033	-58.727	-22.170	4.845
1100	18.489	44.579	31.971	13.869	-58.445	-18.525	3.681
1113	18.524	44.797	32.120	14.110	-58.408	-18.054	3.545
1113	23.900	48.297	32.120	18.005	-54.513	-18.054	3.545
1200	23.900	50.096	33.359	20.084	-53.808	-15.229	2.774
1210.4	23.900	50.302	33.504	20.333	-53.725	-14.891	2.689
1210.4	23.900	50.302	33.504	20.333	-62.555	-14.891	2.689
1300	23.900	52.009	34.721	22.474	-61.818	-11.387	1.914
1400	23.900	53.780	36.020	24.864	-61.005	-7.536	1.176
1500	23.900	55.429	37.260	27.254	-60.199	-3.739	.545

*Data above 298 K estimated except temperature and enthalpy of fusion.

Phase changes: 1113 K, melting point of GeS₂; ΔH° = 3.895 kcal/mol.
1210.4 K, melting point of Ge; ΔH° = 8.830 kcal/mol.

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

298.15-1113 K: Cp° = 15.665 + 2.624x10⁻³T - 0.664x10⁻⁵T²
H° - H₂₉₈° = 15.665x10⁻³T + 1.312x10⁻⁶T² + 0.664x10⁻²T⁻¹ - 5.010
1113-1500 K: Cp° = 23.900
H° - H₂₉₈° = 23.900x10⁻³T - 8.596

Reaction equations (kcal/mol):

298.15-1113 K: ΔHr° = -60.986 + 1.741x10⁻³T + 0.526x10⁻⁶T² - 26.800T⁻¹
ΔGr° = -60.986 - 1.741x10⁻³TlnT - 0.526x10⁻⁶T² - 13.400T⁻¹ + 51.389x10⁻³T
1113-1210.4 K: ΔHr° = -64.572 + 9.976x10⁻³T - 0.786x10⁻⁶T² - 93.200T⁻¹
ΔGr° = -64.572 - 9.976x10⁻³TlnT + 0.786x10⁻⁶T² - 46.600T⁻¹ + 110.945x10⁻³T
1210.4-1500 K: ΔHr° = -72.871 + 8.957x10⁻³T - 0.320x10⁻⁶T² - 68.300T⁻¹
ΔGr° = -72.871 - 8.957x10⁻³TlnT + 0.320x10⁻⁶T² - 34.150T⁻¹ + 111.124x10⁻³T

Sources: Enthalpy of formation at 298 K from Murray (84). Other data from Gurvich (49) who estimated all above 298 K except temperature and enthalpy of fusion.

GeS₂(g)
Germanium Disulfide (ideal gas)
[Formation: Ge(c) + 2S(c,l) = GeS₂(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	13.087	63.762	63.762	0	14.900	2.673	-1.959
300	13.103	63.842	63.762	.024	14.894	2.596	-1.891
368.3	13.553	66.584	64.037	.938	14.649	-.179	.106
368.3	13.553	66.584	64.037	.938	14.457	-.179	.106
388.36	13.685	67.307	64.188	1.211	14.376	-.973	.548
388.36	13.685	67.307	64.188	1.211	13.550	-.973	.548
400	13.762	67.712	64.285	1.371	13.466	-1.408	.769
432.02	13.879	68.776	64.578	1.814	13.195	-2.589	1.310
500	14.128	70.826	65.292	2.767	12.398	-5.003	2.187
600	14.347	73.423	66.438	4.191	11.508	-8.393	3.057
700	14.486	75.646	67.597	5.634	10.744	-11.652	3.638
717.824	14.503	76.010	67.802	5.892	10.619	-12.219	3.720

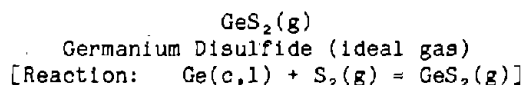
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: $C_p^\circ = 14.653 + 0.150 \times 10^{-3}T - 1.432 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 14.653 \times 10^{-3}T + 0.075 \times 10^{-6}T^2 + 1.432 \times 10^{-2}T^{-1} - 4.856$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 17.446 - 7.276 \times 10^{-3}T + 3.043 \times 10^{-6}T^2 - 192.900T^{-1}$
 $\Delta G_f^\circ = 17.446 + 7.276 \times 10^{-3}T \ln T - 3.043 \times 10^{-6}T^2 - 96.450T^{-1} - 89.012 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = 15.216 - 2.750 \times 10^{-3}T - 0.449 \times 10^{-6}T^2 + 118.300T^{-1}$
 $\Delta G_f^\circ = 15.216 + 2.750 \times 10^{-3}T \ln T + 0.449 \times 10^{-6}T^2 + 59.150T^{-1} - 58.646 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = -17.101 + 86.730 \times 10^{-3}T - 87.013 \times 10^{-6}T^2 + 3922.700T^{-1}$
 $\Delta G_f^\circ = -17.101 - 86.730 \times 10^{-3}T \ln T + 87.013 \times 10^{-6}T^2 + 1961.350T^{-1} + 511.810 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = -36.058 + 78.918 \times 10^{-3}T - 47.389 \times 10^{-6}T^2 + 10375.700T^{-1}$
 $\Delta G_f^\circ = -36.058 - 78.918 \times 10^{-3}T \ln T + 47.389 \times 10^{-6}T^2 + 5187.850T^{-1} + 508.115 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	13.087	63.762	63.762	0	-15.810	-16.354	11.988
300	13.103	63.842	63.762	.024	-15.810	-16.358	11.917
400	13.762	67.712	64.285	1.371	-15.836	-16.539	9.036
500	14.128	70.826	65.292	2.767	-15.857	-16.709	7.304
600	14.347	73.423	66.438	4.191	-15.881	-16.875	6.147
700	14.486	75.646	67.597	5.634	-15.906	-17.042	5.321
800	14.580	77.587	68.728	7.087	-15.938	-17.202	4.699
900	14.645	79.308	69.809	8.549	-15.982	-17.355	4.214
1000	14.693	80.853	70.837	10.016	-16.044	-17.510	3.827
1100	14.729	82.255	71.812	11.487	-16.127	-17.650	3.507
1200	14.756	83.538	72.737	12.961	-16.231	-17.783	3.239
1210.4	14.758	83.665	72.831	13.114	-16.243	-17.792	3.212
1210.4	14.758	83.665	72.831	13.114	-25.073	-17.792	3.212
1300	14.778	84.720	73.615	14.436	-25.156	-17.249	2.900
1400	14.795	85.816	74.447	15.917	-25.252	-16.634	2.597
1500	14.809	86.837	75.239	17.397	-25.356	-16.008	2.332
1600	14.820	87.793	75.994	18.878	-25.466	-15.391	2.102
1700	14.830	88.692	76.715	20.361	-25.582	-14.758	1.897
1800	14.837	89.540	77.404	21.844	-25.703	-14.113	1.714
1900	14.844	90.342	78.064	23.328	-25.830	-13.459	1.548
2000	14.850	91.104	78.697	24.813	-25.962	-12.802	1.399

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: $C_p^\circ = 14.653 + 0.150 \times 10^{-3}T - 1.432 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 14.653 \times 10^{-3}T + 0.075 \times 10^{-6}T^2 + 1.432 \times 10^{-2}T^{-1} - 4.856$

Reaction equations (kcal/mol):

298.15-1210.4 K: $\Delta H_r^\circ = -16.132 + 0.729 \times 10^{-3}T - 0.711 \times 10^{-6}T^2 + 50 T^{-1}$
 $\Delta G_r^\circ = -16.132 - 0.729 \times 10^{-3}T \ln T + 0.711 \times 10^{-6}T^2 + 25.000T^{-1} + 2.914 \times 10^{-3}T$
 1210.4-2000 K: $\Delta H_r^\circ = -24.432 - 0.290 \times 10^{-3}T - 0.245 \times 10^{-6}T^2 + 74.900T^{-1}$
 $\Delta G_r^\circ = -24.432 + 0.290 \times 10^{-3}T \ln T + 0.245 \times 10^{-6}T^2 + 37.450T^{-1} + 3.093 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Karbanov (61). Other data are from Gurvich (49).

HS(g)
Monohydrogen Sulfide (ideal gas)
[Formation: $0.5\text{H}_2(\text{g}) + \text{S}(\text{c},1) = \text{HS}(\text{g})$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H _{2,ss} °)/T	H°- H _{2,ss} °	ΔHf°	ΔGf°	
298.15	7.755	46.730	46.730	0	33.300	26.304	-19.281
300	7.752	46.778	46.731	.014	33.298	26.260	-19.130
368.3	7.633	48.356	46.890	.540	33.203	24.668	-14.638
368.3	7.633	48.356	46.890	.540	33.107	24.668	-14.638
388.36	7.598	48.760	46.976	.693	33.071	24.210	-13.624
388.36	7.598	48.760	46.976	.693	32.658	24.210	-13.624
400	7.578	48.984	47.032	.781	32.617	23.957	-13.089
432.02	7.546	49.566	47.198	1.023	32.485	23.268	-11.771
500	7.477	50.662	47.596	1.533	32.083	21.852	-9.551
600	7.464	52.023	48.225	2.279	31.622	19.850	-7.230
700	7.517	53.177	48.851	3.028	31.220	17.921	-5.595
717.824	7.534	53.366	48.961	3.162	31.154	17.583	-5.353

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta\text{H}^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta\text{H}^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta\text{H}^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2500 K: $\text{Cp}^\circ = 6.851 + 0.916 \times 10^{-3}T + 0.561 \times 10^{-5}T^{-2}$
 $\text{H}^\circ - \text{H}_{2,ss}^\circ = 6.851 \times 10^{-3}T + 0.458 \times 10^{-6}T^2 - 0.561 \times 10^{-2}T^{-1} - 1.895$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta\text{Hf}^\circ = 35.165 - 4.551 \times 10^{-3}T + 1.966 \times 10^{-6}T^2 - 203.450T^{-1}$
 $\Delta\text{Gf}^\circ = 35.165 + 4.551 \times 10^{-3}T \ln T - 1.966 \times 10^{-6}T^2 - 101.725T^{-1} - 53.919 \times 10^{-3}T$
368.3-388.36 K: $\Delta\text{Hf}^\circ = 34.049 - 2.288 \times 10^{-3}T + 0.219 \times 10^{-6}T^2 - 47.850T^{-1}$
 $\Delta\text{Gf}^\circ = 34.049 + 2.288 \times 10^{-3}T \ln T - 0.219 \times 10^{-6}T^2 - 23.925T^{-1} - 38.736 \times 10^{-3}T$
388.36-432.02 K: $\Delta\text{Hf}^\circ = 17.891 + 42.452 \times 10^{-3}T - 43.063 \times 10^{-6}T^2 + 1854.350T^{-1}$
 $\Delta\text{Gf}^\circ = 17.891 - 42.452 \times 10^{-3}T \ln T + 43.063 \times 10^{-6}T^2 + 927.175T^{-1} + 246.493 \times 10^{-3}T$
432.02-717.824 K: $\Delta\text{Hf}^\circ = 8.412 + 38.546 \times 10^{-3}T - 23.251 \times 10^{-6}T^2 + 5080.850T^{-1}$
 $\Delta\text{Gf}^\circ = 8.412 - 38.546 \times 10^{-3}T \ln T + 23.251 \times 10^{-6}T^2 + 2540.425T^{-1} + 244.645 \times 10^{-3}T$

HS(g)
Monohydrogen Sulfide (ideal gas)
[Reaction: $0.5\text{H}_2(\text{g}) + 0.5\text{S}_2(\text{g}) = \text{HS}(\text{g})$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	7.755	46.730	46.730	0	17.945	16.790	-12.307
300	7.752	46.778	46.731	.014	17.945	16.783	-12.226
400	7.578	48.984	47.032	.781	17.966	16.391	-8.956
500	7.477	50.662	47.596	1.533	17.956	15.999	-6.993
600	7.464	52.023	48.225	2.279	17.927	15.609	-5.686
700	7.517	53.177	48.851	3.028	17.895	15.226	-4.754
800	7.611	54.186	49.456	3.784	17.862	14.847	-4.056
900	7.724	55.089	50.033	4.550	17.833	14.471	-3.514
1000	7.843	55.909	50.580	5.329	17.809	14.099	-3.081
1100	7.959	56.662	51.099	6.119	17.789	13.729	-2.728
1200	8.069	57.359	51.592	6.920	17.771	13.361	-2.433
1300	8.170	58.009	52.061	7.732	17.755	12.994	-2.184
1400	8.263	58.618	52.508	8.554	17.741	12.628	-1.971
1500	8.347	59.191	52.934	9.385	17.727	12.263	-1.787
1600	8.422	59.732	53.343	10.223	17.710	11.899	-1.625
1700	8.491	60.245	53.734	11.069	17.694	11.537	-1.483
1800	8.553	60.732	54.109	11.921	17.675	11.175	-1.357
1900	8.609	61.196	54.470	12.779	17.654	10.815	-1.244
2000	8.661	61.639	54.818	13.643	17.632	10.456	-1.143
2100	8.707	62.063	55.153	14.511	17.608	10.096	-1.051
2200	8.750	62.469	55.476	15.384	17.581	9.738	-.967
2300	8.790	62.859	55.789	16.261	17.554	9.383	-.892
2400	8.827	63.234	56.092	17.142	17.524	9.029	-.822
2500	8.860	63.595	56.385	18.026	17.492	8.675	-.758

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

298.15-2500 K: $\text{Cp}^\circ = 6.851 + 0.916 \times 10^{-3}T + 0.561 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 6.851 \times 10^{-3}T + 0.458 \times 10^{-6}T^2 - 0.561 \times 10^{-2}T^{-1} - 1.895$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta\text{Hr}^\circ = 18.376 - 0.549 \times 10^{-3}T + 0.088 \times 10^{-6}T^2 - 82.000T^{-1}$
 $\Delta\text{Gr}^\circ = 18.376 + 0.549 \times 10^{-3}T \ln T - 0.088 \times 10^{-6}T^2 - 41.000T^{-1} - 7.956 \times 10^{-3}T$
2000-2500 K: $\Delta\text{Hr}^\circ = 19.401 - 1.132 \times 10^{-3}T + 0.198 \times 10^{-6}T^2 - 677.850T^{-1}$
 $\Delta\text{Gr}^\circ = 19.401 + 1.132 \times 10^{-3}T \ln T - 0.198 \times 10^{-6}T^2 - 338.925T^{-1} - 12.609 \times 10^{-3}T$

Source: Data from Chase (17).

DS(g)
Monodeuterium Sulfide (ideal gas)
[Formation: $0.5D_2(g) + S(c,l) = DS(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	7.772	48.130	48.130	0	33.100	26.195	-19.201
300	7.770	48.178	48.131	.014	33.097	26.152	-19.052
368.3	7.701	49.762	48.290	.542	33.004	24.581	-14.586
368.3	7.701	49.762	48.290	.542	32.908	24.581	-14.586
388.36	7.681	50.170	48.376	.697	32.873	24.129	-13.578
388.36	7.681	50.170	48.376	.697	32.460	24.129	-13.578
400	7.669	50.397	48.432	.786	32.420	23.880	-13.047
432.02	7.672	50.988	48.600	1.032	32.291	23.200	-11.736
500	7.678	52.107	49.003	1.552	31.899	21.803	-9.530
600	7.770	53.514	49.641	2.324	31.462	19.827	-7.222
700	7.898	54.721	50.282	3.107	31.089	17.917	-5.594
717.824	7.922	54.920	50.395	3.248	31.029	17.583	-5.353

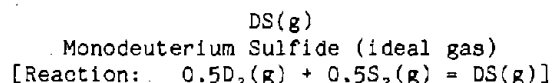
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: $C_p^\circ = 7.096 + 1.054 \times 10^{-3}T + 0.322 \times 10^{-5}T^{-2}$
 $H^\circ - H^\circ_{298} = 7.096 \times 10^{-3}T + 0.527 \times 10^{-6}T^2 - 0.322 \times 10^{-2}T^{-1} - 2.055$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 34.763 - 4.210 \times 10^{-3}T + 1.930 \times 10^{-6}T^2 - 172.750T^{-1}$
 $\Delta G_f^\circ = 34.763 + 4.210 \times 10^{-3}T \ln T - 1.930 \times 10^{-6}T^2 - 86.375T^{-1} - 51.177 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = 33.648 - 1.947 \times 10^{-3}T + 0.183 \times 10^{-6}T^2 - 17.150T^{-1}$
 $\Delta G_f^\circ = 33.648 + 1.947 \times 10^{-3}T \ln T - 0.183 \times 10^{-6}T^2 - 8.575T^{-1} - 35.994 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = 17.490 + 42.793 \times 10^{-3}T - 43.098 \times 10^{-6}T^2 + 1885.050T^{-1}$
 $\Delta G_f^\circ = 17.490 - 42.793 \times 10^{-3}T \ln T + 43.098 \times 10^{-6}T^2 + 942.525T^{-1} + 249.234 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = 8.011 + 38.887 \times 10^{-3}T - 23.287 \times 10^{-6}T^2 + 5111.550T^{-1}$
 $\Delta G_f^\circ = 8.011 - 38.887 \times 10^{-3}T \ln T + 23.287 \times 10^{-6}T^2 + 2555.775T^{-1} + 247.387 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	7.772	48.130	48.130	0	17.745	16.681	-12.228
300	7.770	48.178	48.131	.014	17.745	16.675	-12.147
400	7.669	50.397	48.432	.786	17.769	16.314	-8.913
500	7.678	52.107	49.003	1.552	17.772	15.950	-6.972
600	7.770	53.514	49.641	2.324	17.767	15.586	-5.677
700	7.898	54.721	50.282	3.107	17.764	15.222	-4.752
800	8.034	55.785	50.905	3.904	17.764	14.860	-4.059
900	8.162	56.739	51.501	4.714	17.766	14.495	-3.520
1000	8.277	57.605	52.069	5.536	17.770	14.132	-3.089
1100	8.378	58.398	52.608	6.369	17.774	13.769	-2.736
1200	8.467	59.131	53.122	7.211	17.777	13.405	-2.441
1300	8.544	59.812	53.610	8.062	17.778	13.040	-2.192
1400	8.611	60.448	54.077	8.919	17.776	12.674	-1.979
1500	8.670	61.044	54.521	9.784	17.773	12.311	-1.794
1600	8.722	61.605	54.947	10.653	17.765	11.947	-1.632
1700	8.768	62.135	55.354	11.528	17.755	11.584	-1.489
1800	8.810	62.638	55.745	12.407	17.742	11.221	-1.362
1900	8.847	63.115	56.120	13.290	17.724	10.860	-1.249
2000	8.881	63.570	56.482	14.176	17.704	10.498	-1.147

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

$$298.15-2000 \text{ K: } \begin{aligned} C_p^\circ &= 7.096 + 1.054 \times 10^{-3}T + 0.322 \times 10^{-5}T^2 \\ H^\circ - H_{298}^\circ &= 7.096 \times 10^{-3}T + 0.527 \times 10^{-6}T^2 - 0.322 \times 10^{-2}T^{-1} - 2.055 \end{aligned}$$

Reaction equations (kcal/mol):

$$298.15-2000 \text{ K: } \begin{aligned} \Delta H_r^\circ &= 17.974 - 0.208 \times 10^{-3}T + 0.052 \times 10^{-6}T^2 - 51.300T^{-1} \\ \Delta G_r^\circ &= 17.974 + 0.208 \times 10^{-3}T \ln T - 0.052 \times 10^{-6}T^2 - 25.650T^{-1} - 5.214 \times 10^{-3}T \end{aligned}$$

Source: Data from Chase (17).

$\text{H}_2\text{S(g)}$
Hydrogen Sulfide (ideal gas)
[Formation: $\text{H}_2(\text{g}) + \text{S(c,l)} = \text{H}_2\text{S(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	8.172	49.151	49.151	0	-4.930	-7.996	5.861
300	8.176	49.202	49.152	.015	-4.938	-8.015	5.839
368.3	8.400	50.899	49.321	.581	-5.229	-8.684	5.153
368.3	8.400	50.899	49.321	.581	-5.325	-8.684	5.153
388.36	8.466	51.346	49.415	.750	-5.415	-8.864	4.988
388.36	8.466	51.346	49.415	.750	-5.828	-8.864	4.988
400	8.504	51.597	49.474	.849	-5.898	-8.954	4.892
432.02	8.627	52.257	49.657	1.123	-6.110	-9.191	4.650
500	8.889	53.536	50.100	1.718	-6.665	-9.631	4.210
600	9.306	55.193	50.813	2.628	-7.312	-10.161	3.701
700	9.737	56.660	51.546	3.580	-7.862	-10.592	3.307
717.824	9.813	56.906	51.676	3.754	-7.950	-10.660	3.245

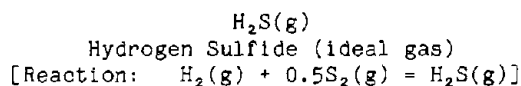
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $C_p^\circ = 7.541 + 3.210 \times 10^{-3}T - 0.290 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 7.541 \times 10^{-3}T + 1.605 \times 10^{-6}T^2 + 0.290 \times 10^{-2}T^{-1} - 2.488$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -2.705 - 7.089 \times 10^{-3}T + 2.903 \times 10^{-6}T^2 - 110.100T^{-1}$
 $\Delta G_f^\circ = -2.705 + 7.089 \times 10^{-3}T \ln T - 2.903 \times 10^{-6}T^2 - 55.050T^{-1} - 56.650 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = -3.820 - 4.826 \times 10^{-3}T + 1.157 \times 10^{-6}T^2 + 45.500T^{-1}$
 $\Delta G_f^\circ = -3.820 + 4.826 \times 10^{-3}T \ln T - 1.157 \times 10^{-6}T^2 + 22.750T^{-1} - 41.468 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = -19.979 + 39.914 \times 10^{-3}T - 42.125 \times 10^{-6}T^2 + 1947.700T^{-1}$
 $\Delta G_f^\circ = -19.979 - 39.914 \times 10^{-3}T \ln T + 42.125 \times 10^{-6}T^2 + 973.850T^{-1} + 243.761 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = -29.457 + 36.008 \times 10^{-3}T - 22.313 \times 10^{-6}T^2 + 5174.200T^{-1}$
 $\Delta G_f^\circ = -29.457 - 36.008 \times 10^{-3}T \ln T + 22.313 \times 10^{-6}T^2 + 2587.100T^{-1} + 241.913 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15	8.172	49.151	49.151	0	-20.285	-17.510	12.835
300	8.176	49.202	49.152	.015	-20.290	-17.492	12.743
400	8.504	51.597	49.474	.849	-20.549	-16.520	9.026
500	8.889	53.536	50.100	1.718	-20.792	-15.485	6.768
600	9.306	55.193	50.813	2.628	-21.007	-14.402	5.246
700	9.737	56.660	51.546	3.580	-21.187	-13.287	4.148
800	10.162	57.988	52.269	4.575	-21.333	-12.148	3.319
900	10.567	59.209	52.973	5.612	-21.448	-10.993	2.669
1000	10.943	60.342	53.655	6.687	-21.534	-9.827	2.148
1100	11.281	61.401	54.311	7.799	-21.596	-8.653	1.719
1200	11.584	62.396	54.944	8.943	-21.639	-7.473	1.361
1300	11.853	63.334	55.553	10.115	-21.667	-6.292	1.058
1400	12.092	64.221	56.141	11.312	-21.684	-5.109	.797
1500	12.303	65.063	56.708	12.532	-21.694	-3.925	.572
1600	12.491	65.863	57.256	13.772	-21.696	-2.741	.374
1700	12.658	66.625	57.784	15.030	-21.694	-1.554	.200
1800	12.808	67.353	58.296	16.303	-21.691	-.370	.045
1900	12.941	68.049	58.791	17.590	-21.685	.814	-.094
2000	13.063	68.716	59.271	18.891	-21.677	1.998	-.218

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

298.15-2000 K: $C_p^\circ = 7.541 + 3.210 \times 10^{-3}T - 0.290 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 7.541 \times 10^{-3}T + 1.605 \times 10^{-6}T^2 + 0.290 \times 10^{-2}T^{-1} - 2.488$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -19.494 - 3.086 \times 10^{-3}T + 1.026 \times 10^{-6}T^2 + 11.350T^{-1}$
 $\Delta G_r^\circ = -19.494 + 3.086 \times 10^{-3}T \ln T - 1.026 \times 10^{-6}T^2 + 5.675T^{-1} - 10.687 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Wagman (126). Other data from Chase (17).

$D_2S(g)$
Deuterium Sulfide (ideal gas)
[Formation: $D_2(g) + S(c,l) = D_2S(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	8.547	51.428	51.428	0	-5.710	-8.437	6.185
300	8.555	51.481	51.428	.016	-5.717	-8.454	6.159
368.3	8.915	53.270	51.609	.612	-5.982	-9.050	5.370
368.3	8.915	53.270	51.609	.612	-6.078	-9.050	5.370
388.36	9.021	53.746	51.707	.792	-6.157	-9.208	5.182
388.36	9.021	53.746	51.707	.792	-6.570	-9.208	5.182
400	9.082	54.013	51.771	.897	-6.634	-9.287	5.074
432.02	9.261	54.719	51.963	1.191	-6.827	-9.492	4.802
500	9.642	56.100	52.432	1.834	-7.334	-9.868	4.313
600	10.199	57.908	53.198	2.826	-7.904	-10.320	3.759
700	10.716	59.520	53.989	3.872	-8.370	-10.686	3.336
717.824	10.797	59.790	54.129	4.064	-8.443	-10.743	3.271

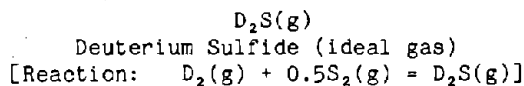
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2500 K: $C_p^\circ = 9.423 + 2.262 \times 10^{-3}T - 1.378 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 9.423 \times 10^{-3}T + 1.131 \times 10^{-6}T^2 + 1.378 \times 10^{-2}T^{-1} - 3.372$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -4.453 - 5.015 \times 10^{-3}T + 2.219 \times 10^{-6}T^2 + 12.300T^{-1}$
 $\Delta G_f^\circ = -4.453 + 5.015 \times 10^{-3}T \ln T - 2.219 \times 10^{-6}T^2 + 6.150T^{-1} - 41.343 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = -5.568 - 2.752 \times 10^{-3}T + 0.473 \times 10^{-6}T^2 + 167.900T^{-1}$
 $\Delta G_f^\circ = -5.568 + 2.752 \times 10^{-3}T \ln T - 0.473 \times 10^{-6}T^2 + 83.950T^{-1} - 26.160 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = -21.727 + 41.988 \times 10^{-3}T - 42.809 \times 10^{-6}T^2 + 2070.100T^{-1}$
 $\Delta G_f^\circ = -21.727 - 41.988 \times 10^{-3}T \ln T + 42.809 \times 10^{-6}T^2 + 1035.050T^{-1} + 259.068 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = -31.205 + 38.082 \times 10^{-3}T - 22.997 \times 10^{-6}T^2 + 5296.600T^{-1}$
 $\Delta G_f^\circ = -31.205 - 38.082 \times 10^{-3}T \ln T + 22.997 \times 10^{-6}T^2 + 2648.300T^{-1} + 257.221 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	8.547	51.428	51.428	0	-21.065	-17.951	13.158
300	8.555	51.481	51.428	.016	-21.069	-17.931	13.063
400	9.082	54.013	51.771	.897	-21.285	-16.852	9.208
500	9.642	56.100	52.432	1.834	-21.461	-15.722	6.872
600	10.199	57.908	53.198	2.826	-21.598	-14.561	5.304
700	10.716	59.520	53.989	3.872	-21.695	-13.381	4.178
800	11.173	60.981	54.772	4.967	-21.759	-12.187	3.329
900	11.589	62.322	55.538	6.106	-21.795	-10.989	2.669
1000	11.909	63.560	56.279	7.281	-21.813	-9.787	2.139
1100	12.196	64.709	56.994	8.487	-21.817	-8.584	1.706
1200	12.440	65.781	57.682	9.719	-21.813	-7.381	1.344
1300	12.649	66.785	58.343	10.974	-21.802	-6.179	1.039
1400	12.828	67.729	58.980	12.248	-21.788	-4.978	.777
1500	12.983	68.619	59.594	13.538	-21.773	-3.778	.550
1600	13.118	69.462	60.185	14.843	-21.755	-2.579	.352
1700	13.236	70.261	60.755	16.161	-21.739	-1.382	.178
1800	13.342	71.020	61.303	17.490	-21.722	-.183	.022
1900	13.434	71.744	61.834	18.829	-21.708	1.013	-.117
2000	13.520	72.435	62.346	20.177	-21.694	2.210	-.241

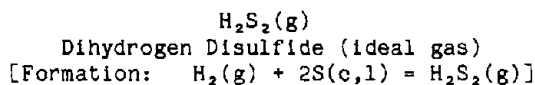
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $C_p^\circ = 9.423 + 2.262 \times 10^{-3}T - 1.378 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 9.423 \times 10^{-3}T + 1.131 \times 10^{-6}T^2 + 1.378 \times 10^{-2}T^{-1} - 3.372$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -21.242 - 1.012 \times 10^{-3}T + 0.342 \times 10^{-6}T^2 + 133.750T^{-1}$
 $\Delta G_r^\circ = -21.242 + 1.012 \times 10^{-3}T \ln T - 0.342 \times 10^{-6}T^2 + 66.875T^{-1} + 4.620 \times 10^{-3}T$

Source: Data from Chase (17).



T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	12.300	63.660	63.660	0	3.760	-1.348	.988
300	12.320	63.740	63.663	.023	3.750	-1.380	1.005
368.3	12.921	66.332	63.918	.889	3.375	-2.506	1.487
368.3	12.921	66.332	63.918	.889	3.183	-2.506	1.487
388.36	13.098	67.022	64.061	1.150	3.066	-2.812	1.582
388.36	13.098	67.022	64.061	1.150	2.240	-2.812	1.582
400	13.200	67.410	64.153	1.303	2.136	-2.962	1.618
432.02	13.395	68.434	64.432	1.729	1.812	-3.359	1.699
500	13.810	70.420	65.112	2.654	.914	-4.096	1.790
600	14.320	72.990	66.222	4.061	-.093	-5.003	1.822
700	14.780	75.230	67.349	5.517	-.939	-5.751	1.795
717.824	14.858	75.603	67.549	5.781	-1.074	-5.871	1.787

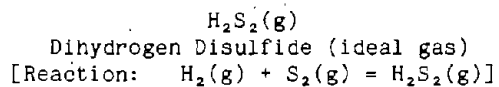
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-1000 K: $C_p^\circ = 12.280 + 3.866 \times 10^{-3}T - 1.005 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 12.280 \times 10^{-3}T + 1.933 \times 10^{-6}T^2 + 1.005 \times 10^{-2}T^{-1} - 4.170$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 7.109 - 10.524 \times 10^{-3}T + 4.948 \times 10^{-6}T^2 - 194.200T^{-1}$
 $\Delta G_f^\circ = 7.109 + 10.524 \times 10^{-3}T \ln T - 4.948 \times 10^{-6}T^2 - 97.100T^{-1} - 85.758 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = 4.879 - 5.998 \times 10^{-3}T + 1.456 \times 10^{-6}T^2 + 117.000T^{-1}$
 $\Delta G_f^\circ = 4.879 + 5.998 \times 10^{-3}T \ln T - 1.456 \times 10^{-6}T^2 + 58.500T^{-1} - 55.392 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -27.438 + 83.482 \times 10^{-3}T - 85.108 \times 10^{-6}T^2 + 3921.400T^{-1}$
 $\Delta G_f^\circ = -27.438 - 83.482 \times 10^{-3}T \ln T + 85.108 \times 10^{-6}T^2 + 1960.700T^{-1} + 515.064 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -46.395 + 75.670 \times 10^{-3}T - 45.484 \times 10^{-6}T^2 + 10374.400T^{-1}$
 $\Delta G_f^\circ = -46.395 - 75.670 \times 10^{-3}T \ln T + 45.484 \times 10^{-6}T^2 + 5187.200T^{-1} + 511.369 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/T$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔH°	ΔG°	
298.15	12.300	63.660	63.660	0	-26.950	-20.375	14.935
300	12.320	63.740	63.663	.023	-26.954	-20.335	14.813
400	13.200	67.410	64.153	1.303	-27.166	-18.093	9.886
500	13.810	70.420	65.112	2.654	-27.341	-15.802	6.907
600	14.320	72.990	66.222	4.061	-27.482	-13.485	4.912
700	14.780	75.230	67.349	5.517	-27.589	-11.141	3.478
800	15.220	77.230	68.459	7.017	-27.666	-8.783	2.399
900	15.630	79.050	69.540	8.559	-27.715	-6.425	1.560
1000	16.050	80.720	70.576	10.144	-27.735	-4.058	.887

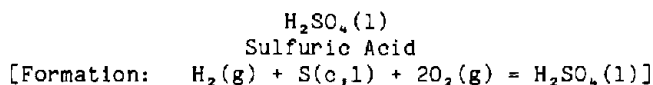
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $\text{Cp}^\circ = 12.280 + 3.866 \times 10^{-3}T - 1.005 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 12.280 \times 10^{-3}T + 1.933 \times 10^{-6}T^2 + 1.005 \times 10^{-2}T^{-1} - 4.170$

Reaction equations (kcal/mol):

298.15-1000 K: $\Delta \text{H}^\circ = -26.468 - 2.519 \times 10^{-3}T + 1.194 \times 10^{-6}T^2 + 48.700T^{-1}$
 $\Delta \text{G}^\circ = -26.468 + 2.519 \times 10^{-3}T \ln T - 1.194 \times 10^{-6}T^2 + 24.350T^{-1} + 6.168 \times 10^{-3}T$

Source: Data from Mills (80).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/T$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHf°	ΔGf°	
298.15	33.125	37.501	37.501	0	-194.548	-164.919	120.887
300	33.210	37.706	37.503	.061	-194.536	-164.735	120.008
368.3	36.355	44.828	38.213	2.436	-193.983	-158.006	93.760
368.3	36.355	44.828	38.213	2.436	-194.079	-158.006	93.760
388.36	37.279	46.781	38.606	3.175	-193.887	-156.046	87.814
388.36	37.279	46.781	38.606	3.175	-194.300	-156.046	87.814
400	37.815	47.890	38.860	3.612	-194.199	-154.901	84.633
432.02	39.301	50.859	39.641	4.847	-193.914	-151.767	76.775
500	42.456	56.826	41.574	7.626	-193.283	-145.174	63.454
600	47.096	64.977	44.805	12.103	-191.873	-135.676	49.419
700	51.737	72.586	48.236	17.045	-189.989	-126.453	39.480

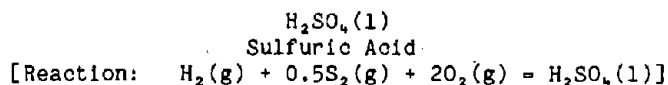
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta\text{H}^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta\text{H}^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta\text{H}^\circ = 0$ kcal/mol.
 610 K, calculated boiling point for $\text{H}_2\text{SO}_4(1) = \text{H}_2\text{SO}_4(\text{g})$; $\Delta\text{H}^\circ = 13.9$ kcal/mol.
 Experimental vapor pressure equals 1 atm at 553 K. The vapor at this temperature is 76.6 mol pct $\text{SO}_3(\text{g})$.

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

298.15-700 K: $\text{Cp}^\circ = 19.153 + 46.528 \times 10^{-3}T + 0.089 \times 10^{-5}T^{-2}$
 $\text{H}^\circ - \text{H}_{298}^\circ = 19.153 \times 10^{-3}T + 23.264 \times 10^{-6}T^2 - 0.089 \times 10^{-2}T^{-1} - 7.749$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta\text{Hf}^\circ = -192.880 - 9.937 \times 10^{-3}T + 23.556 \times 10^{-6}T^2 - 238.400T^{-1}$
 $\Delta\text{Gf}^\circ = -192.880 + 9.937 \times 10^{-3}T \ln T - 23.556 \times 10^{-6}T^2 - 119.200T^{-1} + 45.529 \times 10^{-3}T$
 368.3-388.36 K: $\Delta\text{Hf}^\circ = -193.995 - 7.674 \times 10^{-3}T + 21.810 \times 10^{-6}T^2 - 82.800T^{-1}$
 $\Delta\text{Gf}^\circ = -193.995 + 7.674 \times 10^{-3}T \ln T - 21.810 \times 10^{-6}T^2 - 41.400T^{-1} + 60.711 \times 10^{-3}T$
 388.36-432.02 K: $\Delta\text{Hf}^\circ = -210.153 + 37.066 \times 10^{-3}T - 21.472 \times 10^{-6}T^2 + 1819.400T^{-1}$
 $\Delta\text{Gf}^\circ = -210.153 - 37.066 \times 10^{-3}T \ln T + 21.472 \times 10^{-6}T^2 + 909.700T^{-1} + 345.940 \times 10^{-3}T$
 432.02-700 K: $\Delta\text{Hf}^\circ = -219.632 + 33.160 \times 10^{-3}T - 1.660 \times 10^{-6}T^2 + 5045.900T^{-1}$
 $\Delta\text{Gf}^\circ = -219.632 - 33.160 \times 10^{-3}T \ln T + 1.660 \times 10^{-6}T^2 + 2522.950T^{-1} + 344.092 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15	33.125	37.501	37.501	0	-209.903	-174.432	127.861
300	33.210	37.706	37.503	.061	-209.888	-174.212	126.912
400	37.815	47.890	38.860	3.612	-208.850	-162.466	88.766
500	42.456	56.826	41.574	7.626	-207.410	-151.027	66.013
600	47.096	64.977	44.805	12.103	-205.568	-139.917	50.964
700	51.737	72.586	48.236	17.045	-203.314	-129.148	40.321

Phase change: 610 K, calculated boiling point for $\text{H}_2\text{SO}_4(1) = \text{H}_2\text{SO}_4(\text{g})$; $\Delta H^\circ = 13.9$ kcal/mol.
 Experimental vapor pressure equals 1 atm at 553 K. The vapor at this temperature is 76.6 mol pct $\text{SO}_3(\text{g})$.

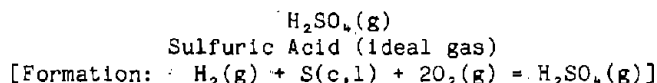
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $C_p^\circ = 19.153 + 46.528 \times 10^{-3}T + 0.089 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 19.153 \times 10^{-3}T + 23.264 \times 10^{-6}T^2 - 0.089 \times 10^{-2}T^3 - 7.749$

Reaction equations (kcal/mol):

298.15-700 K: $\Delta H_r^\circ = -209.669 - 5.934 \times 10^{-3}T + 21.679 \times 10^{-6}T^2 - 116.950T^{-1}$
 $\Delta G_r^\circ = -209.669 + 5.934 \times 10^{-3}T \ln T - 21.679 \times 10^{-6}T^2 - 58.475T^{-1} + 91.491 \times 10^{-3}T$

Source: Data from Chase (17).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHf°	ΔGf°	
298.15*	20.019	71.388	71.388	0	-175.700	-156.174	114.477
300	20.089	71.512	71.389	.037	-175.712	-156.053	113.683
368.3	22.339	75.877	71.820	1.494	-176.078	-151.535	89.920
368.3	22.339	75.877	71.820	1.494	-176.174	-151.535	89.920
388.36	23.000	77.080	72.061	1.949	-176.265	-150.190	84.519
388.36	23.000	77.080	72.061	1.949	-176.678	-150.190	84.519
400	23.383	77.765	72.217	2.219	-176.744	-149.396	81.625
432.02	24.167	79.596	72.697	2.980	-176.932	-147.200	74.464
500	25.831	83.259	73.889	4.685	-177.376	-142.483	62.278
600	27.644	88.137	75.864	7.364	-177.764	-135.463	49.342
700	29.018	92.506	77.935	10.200	-177.986	-128.394	40.086
717.824	29.210	93.238	78.305	10.719	-178.011	-127.130	38.706

*Data except enthalpy of formation at 298 K estimated.

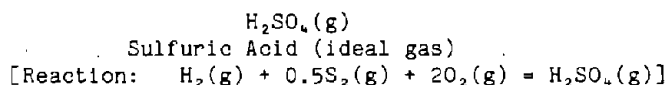
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta\text{H}^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta\text{H}^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta\text{H}^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $\text{Cp}^\circ = 26.093 + 5.712 \times 10^{-3}T - 6.913 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 26.093 \times 10^{-3}T + 2.856 \times 10^{-6}T^2 + 6.913 \times 10^{-2}T^{-1} - 10.352$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta\text{Hf}^\circ = -176.635 - 2.997 \times 10^{-3}T + 3.148 \times 10^{-6}T^2 + 461.800T^{-1}$
 $\Delta\text{Gf}^\circ = -176.635 + 2.997 \times 10^{-3}T \ln T - 3.148 \times 10^{-6}T^2 + 230.900T^{-1} + 49.892 \times 10^{-3}T$
 368.3-388.36 K: $\Delta\text{Hf}^\circ = -177.750 - 0.734 \times 10^{-3}T + 1.402 \times 10^{-6}T^2 + 617.400T^{-1}$
 $\Delta\text{Gf}^\circ = -177.750 + 0.734 \times 10^{-3}T \ln T - 1.402 \times 10^{-6}T^2 + 308.700T^{-1} + 65.075 \times 10^{-3}T$
 388.36-432.02 K: $\Delta\text{Hf}^\circ = -193.909 + 44.006 \times 10^{-3}T - 41.880 \times 10^{-6}T^2 + 2519.600T^{-1}$
 $\Delta\text{Gf}^\circ = -193.909 - 44.006 \times 10^{-3}T \ln T + 41.880 \times 10^{-6}T^2 + 1259.800T^{-1} + 350.303 \times 10^{-3}T$
 432.02-717.824 K: $\Delta\text{Hf}^\circ = -203.387 + 40.100 \times 10^{-3}T - 22.068 \times 10^{-6}T^2 + 5746.100T^{-1}$
 $\Delta\text{Gf}^\circ = -203.387 - 40.100 \times 10^{-3}T \ln T + 22.068 \times 10^{-6}T^2 + 2873.050T^{-1} + 348.456 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15*	20.019	71.388	71.388	0	-191.055	-165.688	121.451
300	20.089	71.512	71.389	.037	-191.064	-165.530	120.587
400	23.383	77.765	72.217	2.219	-191.395	-156.961	85.759
500	25.831	83.259	73.889	4.685	-191.503	-148.336	64.837
600	27.644	88.137	75.864	7.364	-191.458	-139.704	50.887
700	29.018	92.506	77.935	10.200	-191.311	-131.089	40.927
800	30.098	96.454	80.008	13.157	-191.092	-122.502	33.466
900	30.978	100.051	82.037	16.213	-190.814	-113.944	27.669
1000	31.714	103.354	84.006	19.348	-190.495	-105.421	23.039
1100	32.341	106.407	85.905	22.552	-190.143	-96.928	19.258
1200	32.883	109.245	87.733	25.814	-189.764	-88.470	16.112
1300	33.355	111.896	89.491	29.126	-189.364	-80.046	13.457
1400	33.768	114.384	91.182	32.483	-188.949	-71.653	11.185
1500	34.131	116.726	92.807	35.878	-188.524	-63.291	9.221
1600	34.451	118.939	94.372	39.307	-188.091	-54.957	7.507
1700	34.734	121.036	95.879	42.767	-187.652	-46.646	5.997
1800	34.986	123.029	97.333	46.253	-187.211	-38.364	4.658
1900	35.209	124.927	98.736	49.763	-186.770	-30.108	3.463
2000	35.409	126.738	100.091	53.294	-186.331	-21.874	2.390

*Data except enthalpy of formation at 298 K estimated.

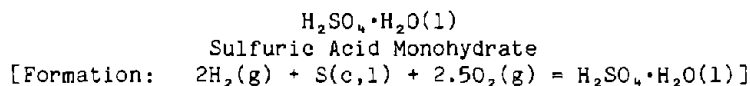
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 26.093 + 5.712 \times 10^{-3}T - 6.913 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 26.093 \times 10^{-3}T + 2.856 \times 10^{-6}T^2 + 6.913 \times 10^{-2}T^{-1} - 10.352$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -193.424 + 1.006 \times 10^{-3}T + 1.271 \times 10^{-6}T^2 + 583.250T^{-1}$
 $\Delta G_r^\circ = -193.424 - 1.006 \times 10^{-3}T \ln T - 1.271 \times 10^{-6}T^2 + 291.625T^{-1} + 95.855 \times 10^{-3}T$

Source: Data from Chase (17) who estimated most molecular constants.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	51.214	50.555	50.555	0	-269.508	-227.161	166.511
300	51.276	50.872	50.555	.095	-269.482	-226.898	165.293
368.3	53.564	61.616	51.637	3.675	-268.439	-217.311	128.951
368.3	53.564	61.616	51.637	3.675	-268.535	-217.311	128.951
388.36	54.236	64.475	52.227	4.756	-268.211	-214.530	120.725
388.36	54.236	64.475	52.227	4.756	-268.624	-214.530	120.725
400	54.626	66.082	52.607	5.390	-268.449	-212.911	116.328
432.02	55.779	70.333	53.765	7.158	-267.971	-208.485	105.467
500	58.227	78.658	56.592	11.033	-266.969	-199.192	87.066
600	61.827	89.592	61.200	17.035	-265.111	-185.806	67.679
700	65.427	99.393	65.967	23.398	-262.897	-172.758	53.937
717.824	66.069	101.046	66.818	24.570	-262.466	-170.468	51.901

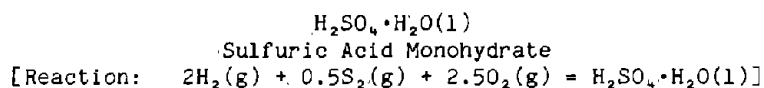
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-1000 K: $\text{Cp}^\circ = 39.876 + 36.338 \times 10^{-3}T + 0.448 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 39.876 \times 10^{-3}T + 18.169 \times 10^{-6}T^2 - 0.448 \times 10^{-2}T^{-1} - 13.354$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta \text{Hf}^\circ = -270.362 + 0.715 \times 10^{-3}T + 17.791 \times 10^{-6}T^2 - 280.400T^{-1}$
 $\Delta \text{Gf}^\circ = -270.362 - 0.715 \times 10^{-3}T \ln T - 17.791 \times 10^{-6}T^2 - 140.200T^{-1} + 155.853 \times 10^{-3}T$
 368.3-388.36 K: $\Delta \text{Hf}^\circ = -271.477 + 2.978 \times 10^{-3}T + 16.045 \times 10^{-6}T^2 - 124.800T^{-1}$
 $\Delta \text{Gf}^\circ = -271.477 - 2.978 \times 10^{-3}T \ln T - 16.045 \times 10^{-6}T^2 - 62.400T^{-1} + 171.036 \times 10^{-3}T$
 388.36-432.02 K: $\Delta \text{Hf}^\circ = -287.636 + 47.718 \times 10^{-3}T - 27.237 \times 10^{-6}T^2 + 1777.400T^{-1}$
 $\Delta \text{Gf}^\circ = -287.636 - 47.718 \times 10^{-3}T \ln T + 27.237 \times 10^{-6}T^2 + 888.700T^{-1} + 456.264 \times 10^{-3}T$
 432.02-717.824 K: $\Delta \text{Hf}^\circ = -297.114 + 43.812 \times 10^{-3}T - 7.425 \times 10^{-6}T^2 + 5003.900T^{-1}$
 $\Delta \text{Gf}^\circ = -297.114 - 43.812 \times 10^{-3}T \ln T + 7.425 \times 10^{-6}T^2 + 2501.950T^{-1} + 454.417 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log K _r
	C _p ^o	S ^o	-(G ^o - H ₂₉₈ ^o)/T	H ^o - H ₂₉₈ ^o	ΔH _r ^o	ΔG _r ^o	
298.15	51.214	50.555	50.555	0	-284.863	-236.675	173.485
300	51.276	50.872	50.555	.095	-284.833	-236.375	172.197
400	54.626	66.082	52.607	5.390	-283.100	-220.477	120.461
500	58.227	78.658	56.592	11.033	-281.096	-205.045	89.624
600	61.827	89.592	61.200	17.035	-278.806	-190.046	69.223
700	65.427	99.393	65.967	23.398	-276.223	-175.453	54.778
800	69.028	108.365	70.714	30.121	-273.342	-161.252	44.051
900	72.628	116.703	75.366	37.203	-270.157	-147.430	35.800
1000	76.228	124.542	79.896	44.646	-266.661	-133.979	29.281

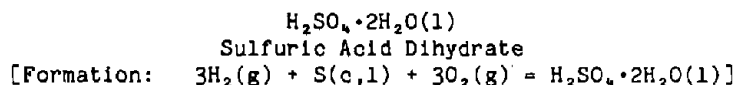
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $C_p^o = 39.876 + 36.338 \times 10^{-3}T + 0.448 \times 10^{-5}T^2$
 $H^o - H_{298}^o = 39.876 \times 10^{-3}T + 18.169 \times 10^{-6}T^2 - 0.448 \times 10^{-2}T^{-1} - 13.354$

Reaction equations (kcal/mol):

298.15-1000 K: $\Delta H_r^o = -287.151 + 4.717 \times 10^{-3}T + 15.914 \times 10^{-6}T^2 - 158.950T^{-1}$
 $\Delta G_r^o = -287.151 - 4.717 \times 10^{-3}T \ln T - 15.914 \times 10^{-6}T^2 - 79.475T^{-1} + 201.816 \times 10^{-3}T$

Source: Data from Chase (17).



T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	62.493	66.056	66.056	0	-341.085	-286.750	210.191
300	62.637	66.443	66.056	.116	-341.057	-286.412	208.649
368.3	67.951	79.816	67.394	4.575	-339.850	-274.094	162.646
368.3	67.951	79.816	67.394	4.575	-339.946	-274.094	162.646
388.36	69.511	83.462	68.132	5.954	-339.536	-270.517	152.232
388.36	69.511	83.462	68.132	5.954	-339.949	-270.517	152.232
400	70.417	85.528	68.608	6.768	-339.717	-268.440	146.667
432.02	72.908	91.047	70.069	9.063	-339.050	-262.761	132.924
500	78.198	102.077	73.679	14.199	-337.513	-250.862	109.650
600	85.979	117.022	79.675	22.408	-334.526	-233.800	85.160
700	93.759	130.860	86.010	31.395	-330.779	-217.298	67.843
717.824	95.146	133.234	87.153	33.078	-330.031	-214.418	65.282

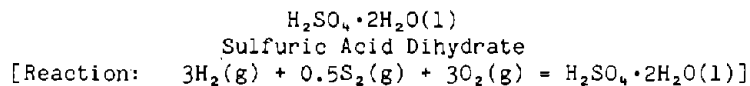
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-1000 K: $C_p^\circ = 39.283 + 77.822 \times 10^{-3}T + 0.006 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 39.283 \times 10^{-3}T + 38.911 \times 10^{-6}T^2 - 0.006 \times 10^{-2}T^3 - 15.169$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -340.672 - 9.949 \times 10^{-3}T + 37.862 \times 10^{-6}T^2 - 242.300T^{-1}$
 $\Delta G_f^\circ = -340.672 + 9.949 \times 10^{-3}T \ln T - 37.862 \times 10^{-6}T^2 - 121.150T^{-1} + 136.821 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -341.787 - 7.686 \times 10^{-3}T + 36.116 \times 10^{-6}T^2 - 86.700T^{-1}$
 $\Delta G_f^\circ = -341.787 + 7.686 \times 10^{-3}T \ln T - 36.116 \times 10^{-6}T^2 - 43.350T^{-1} + 152.004 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -357.945 + 37.054 \times 10^{-3}T - 7.166 \times 10^{-6}T^2 + 1815.500T^{-1}$
 $\Delta G_f^\circ = -357.945 - 37.054 \times 10^{-3}T \ln T + 7.166 \times 10^{-6}T^2 + 907.750T^{-1} + 437.232 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -367.424 + 33.148 \times 10^{-3}T + 12.646 \times 10^{-6}T^2 + 5042.000T^{-1}$
 $\Delta G_f^\circ = -367.424 - 33.148 \times 10^{-3}T \ln T - 12.646 \times 10^{-6}T^2 + 2521.000T^{-1} + 435.384 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH°	ΔG°	
298.15	62.493	66.056	66.056	0	-356.440	-296.263	217.164
300	62.637	66.443	66.056	.116	-356.409	-295.890	215.553
400	70.417	85.528	68.608	6.768	-354.368	-276.006	150.801
500	78.198	102.077	73.679	14.199	-351.640	-256.716	112.209
600	85.979	117.022	79.675	22.408	-348.220	-238.041	86.705
700	93.759	130.860	86.010	31.395	-344.104	-219.993	68.684
800	101.540	143.888	92.438	41.160	-339.286	-202.585	55.343
900	109.320	156.297	98.849	51.703	-333.758	-185.823	45.123
1000	117.101	168.217	105.193	63.024	-327.516	-169.714	37.091

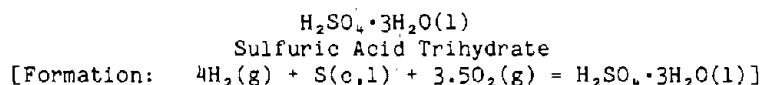
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $\text{Cp}^\circ = 39.283 + 77.822 \times 10^{-3}T + 0.006 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 39.283 \times 10^{-3}T + 38.911 \times 10^{-6}T^2 - 0.006 \times 10^{-2}T^3 - 15.169$

Reaction equations (kcal/mol):

298.15-1000 K: $\Delta H^\circ = -357.461 - 5.947 \times 10^{-3}T + 35.985 \times 10^{-6}T^2 - 120.850T^{-1}$
 $\Delta G^\circ = -357.461 + 5.947 \times 10^{-3}T \ln T - 35.985 \times 10^{-6}T^2 - 60.425T^{-1} + 182.784 \times 10^{-3}T$

Source: Data from Chase (17).



T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	76.270	82.550	82.550	0	-411.186	-345.159	253.005
300	76.325	83.022	82.552	.141	-411.153	-344.749	251.146
368.3	80.971	99.103	84.164	5.502	-409.758	-329.773	195.685
368.3	80.971	99.103	84.164	5.502	-409.854	-329.773	195.685
388.36	82.335	103.435	85.050	7.140	-409.396	-325.423	183.130
388.36	82.335	103.435	85.050	7.140	-409.809	-325.423	183.130
400	83.127	105.878	85.620	8.103	-409.552	-322.898	176.421
432.02	85.333	112.364	87.365	10.800	-408.822	-315.990	159.851
500	90.017	125.168	91.648	16.760	-407.186	-301.498	131.783
600	96.908	142.189	98.677	26.107	-404.139	-280.634	102.220
700	103.798	157.645	106.014	36.142	-400.435	-260.334	81.279
717.824	105.026	160.270	107.328	38.003	-399.705	-256.777	78.178

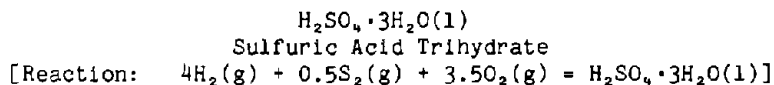
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-1000 K: $C_p^\circ = 54.643 + 70.012 \times 10^{-3}T + 0.669 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 54.643 \times 10^{-3}T + 35.006 \times 10^{-6}T^2 - 0.669 \times 10^{-2}T^{-1} - 19.179$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -411.700 - 4.660 \times 10^{-3}T + 33.286 \times 10^{-6}T^2 - 314.700T^{-1}$
 $\Delta G_f^\circ = -411.700 + 4.660 \times 10^{-3}T \ln T - 33.286 \times 10^{-6}T^2 - 157.350T^{-1} + 208.324 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -412.815 - 2.397 \times 10^{-3}T + 31.541 \times 10^{-6}T^2 - 159.100T^{-1}$
 $\Delta G_f^\circ = -412.815 + 2.397 \times 10^{-3}T \ln T - 31.541 \times 10^{-6}T^2 - 79.550T^{-1} + 223.507 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -428.974 + 42.343 \times 10^{-3}T - 11.741 \times 10^{-6}T^2 + 1743.100T^{-1}$
 $\Delta G_f^\circ = -428.974 - 42.343 \times 10^{-3}T \ln T + 11.741 \times 10^{-6}T^2 + 871.550T^{-1} + 508.736 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -438.452 + 38.437 \times 10^{-3}T + 8.070 \times 10^{-6}T^2 + 4969.600T^{-1}$
 $\Delta G_f^\circ = -438.452 - 38.437 \times 10^{-3}T \ln T - 8.070 \times 10^{-6}T^2 + 2484.800T^{-1} + 506.888 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15	76.270	82.550	82.550	0	-426.541	-354.672	259.979
300	76.325	83.022	82.552	.141	-426.505	-354.226	258.050
400	83.127	105.878	85.620	8.103	-424.203	-330.464	180.555
500	90.017	125.168	91.648	16.760	-421.314	-307.351	134.341
600	96.908	142.189	98.677	26.107	-417.833	-284.875	103.764
700	103.798	157.645	106.014	36.142	-413.760	-263.030	82.120
800	110.689	171.955	113.373	46.866	-409.088	-241.811	66.059
900	117.579	185.390	120.634	58.280	-403.807	-221.212	53.717
1000	124.470	198.135	127.753	70.382	-397.915	-201.236	43.980

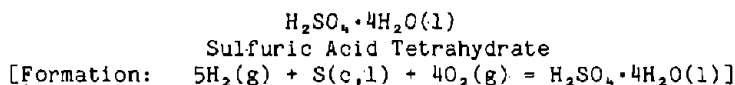
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $C_p^\circ = 54.643 + 70.012 \times 10^{-3}T + 0.669 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 54.643 \times 10^{-3}T + 35.006 \times 10^{-6}T^2 - 0.669 \times 10^{-2}T^3 - 19.179$

Reaction equations (kcal/mol):

298.15-1000 K: $\Delta H_r^\circ = -428.489 - 0.657 \times 10^{-3}T + 31.410 \times 10^{-6}T^2 - 193.250T^{-1}$
 $\Delta G_r^\circ = -428.489 + 0.657 \times 10^{-3}T \ln T - 31.410 \times 10^{-6}T^2 - 96.625T^{-1} + 254.287 \times 10^{-3}T$

Source: Data from Chase (17).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	92.354	99.079	99.079	0	-480.688	-402.979	295.388
300	92.447	99.651	99.081	.171	-480.644	-402.497	293.215
368.3	96.295	118.977	101.029	6.610	-478.886	-384.888	228.390
368.3	96.295	118.977	101.029	6.610	-478.982	-384.888	228.390
388.36	97.425	124.114	102.090	8.553	-478.431	-379.777	213.717
388.36	97.425	124.114	102.090	8.553	-478.844	-379.777	213.717
400	98.081	127.001	102.773	9.691	-478.534	-376.813	205.878
432.02	99.932	134.625	104.855	12.861	-477.670	-368.704	186.517
500	103.861	149.508	109.930	19.789	-475.792	-351.690	153.722
600	109.642	168.955	118.182	30.464	-472.494	-327.171	119.170
700	115.422	186.290	126.694	41.717	-468.663	-303.246	94.676
717.824	116.452	189.204	128.210	43.783	-467.924	-299.044	91.047

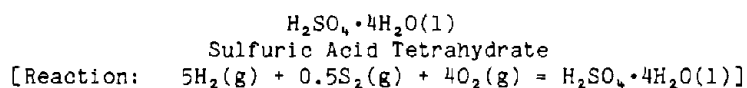
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-1000 K: $\text{Cp}^\circ = 74.381 + 58.476 \times 10^{-3}T + 0.479 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 74.381 \times 10^{-3}T + 29.238 \times 10^{-6}T^2 - 0.479 \times 10^{-3}T^3 - 24.615$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta \text{Hf}^\circ = -483.555 + 5.007 \times 10^{-3}T + 26.848 \times 10^{-6}T^2 - 301.800T^{-1}$
 $\Delta \text{Gf}^\circ = -483.555 - 5.007 \times 10^{-3}T \ln T - 26.848 \times 10^{-6}T^2 - 150.900T^{-1} + 308.484 \times 10^{-3}T$
 368.3-388.36 K: $\Delta \text{Hf}^\circ = -484.670 + 7.270 \times 10^{-3}T + 25.102 \times 10^{-6}T^2 - 146.200T^{-1}$
 $\Delta \text{Gf}^\circ = -484.670 - 7.270 \times 10^{-3}T \ln T - 25.102 \times 10^{-6}T^2 - 73.100T^{-1} + 323.667 \times 10^{-3}T$
 388.36-432.02 K: $\Delta \text{Hf}^\circ = -500.829 + 52.010 \times 10^{-3}T - 18.180 \times 10^{-6}T^2 + 1756.000T^{-1}$
 $\Delta \text{Gf}^\circ = -500.829 - 52.010 \times 10^{-3}T \ln T + 18.180 \times 10^{-6}T^2 + 878.000T^{-1} + 608.895 \times 10^{-3}T$
 432.02-717.824 K: $\Delta \text{Hf}^\circ = -510.307 + 48.104 \times 10^{-3}T + 1.632 \times 10^{-6}T^2 + 4982.500T^{-1}$
 $\Delta \text{Gf}^\circ = -510.307 - 48.104 \times 10^{-3}T \ln T - 1.632 \times 10^{-6}T^2 + 2491.250T^{-1} + 607.047 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15	92.354	99.079	99.079	0	-496.043	-412.493	302.361
300	92.447	99.651	99.081	.171	-495.996	-411.974	300.119
400	98.081	127.001	102.773	9.691	-493.185	-384.378	210.012
500	103.861	149.508	109.930	19.789	-489.919	-357.544	156.280
600	109.642	168.955	118.182	30.464	-486.189	-331.412	120.715
700	115.422	186.290	126.694	41.717	-481.988	-305.941	95.518
800	121.202	202.080	135.145	53.548	-477.314	-281.108	76.794
900	126.983	216.689	143.403	65.957	-472.156	-256.887	62.380
1000	132.763	230.367	151.422	78.945	-466.510	-233.268	50.980

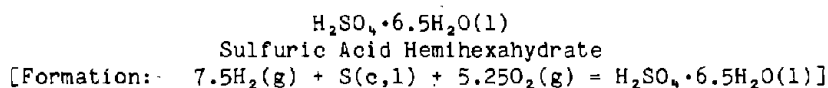
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $C_p^\circ = 74.381 + 58.476 \times 10^{-3}T + 0.479 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 74.381 \times 10^{-3}T + 29.238 \times 10^{-6}T^2 - 0.479 \times 10^{-2}T^{-1} - 24.615$

Reaction equations (kcal/mol):

298.15-1000 K: $\Delta H_r^\circ = -500.344 + 9.009 \times 10^{-3}T + 24.971 \times 10^{-6}T^2 - 180.350T^{-1}$
 $\Delta G_r^\circ = -500.344 - 9.009 \times 10^{-3}T \ln T - 24.971 \times 10^{-6}T^2 - 90.175T^{-1} + 354.447 \times 10^{-3}T$

Source: Data from Chase (17).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	136.309	140.498	140.498	0	-653.265	-546.381	400.503
300	136.389	141.342	140.502	.252	-653.189	-545.718	397.550
368.3	138.452	169.522	143.351	9.639	-650.270	-521.556	309.488
368.3	138.452	169.522	143.351	9.639	-650.366	-521.556	309.488
388.36	139.057	176.881	144.895	12.422	-649.502	-514.563	289.567
388.36	139.057	176.881	144.895	12.422	-649.915	-514.563	289.567
400	139.409	180.993	145.885	14.043	-649.430	-510.514	278.928
432.02	140.373	191.766	148.892	18.522	-648.106	-499.446	252.656
500	142.419	212.425	156.157	28.134	-645.357	-476.255	208.168
600	145.429	238.657	167.780	42.526	-641.035	-442.838	161.301
700	148.439	261.301	179.558	57.220	-636.491	-410.160	128.056
717.824	148.976	265.039	181.634	59.870	-635.658	-404.409	123.126

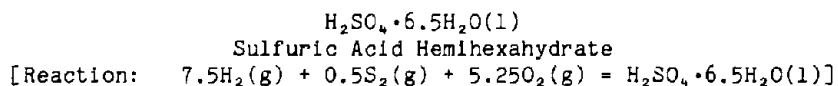
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1000 K: Cp° = 127.506 + 29.940x10⁻³T - 0.110x10⁻⁵T²
 H°- H₂₉₈° = 127.506x10⁻³T + 14.970x10⁻⁶T² + 0.110x10⁻²T⁻¹ - 39.384

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -663.194 + 32.955x10⁻³T + 10.904x10⁻⁶T² - 258.150T⁻¹
 ΔGf° = -663.194 - 32.955x10⁻³TlnT - 10.904x10⁻⁶T² - 129.075T⁻¹ + 584.258x10⁻³T
 368.3-388.36 K: ΔHf° = -664.309 + 35.218x10⁻³T + 9.158x10⁻⁶T² - 102.550T⁻¹
 ΔGf° = -664.309 - 35.218x10⁻³TlnT - 9.158x10⁻⁶T² - 51.275T⁻¹ + 599.440x10⁻³T
 388.36-432.02 K: ΔHf° = -680.467 + 79.958x10⁻³T - 34.124x10⁻⁶T² + 1799.650T⁻¹
 ΔGf° = -680.467 - 79.958x10⁻³TlnT + 34.124x10⁻⁶T² + 899.825T⁻¹ + 884.669x10⁻³T
 432.02-717.824 K: ΔHf° = -689.946 + 76.052x10⁻³T - 14.312x10⁻⁶T² + 5026.150T⁻¹
 ΔGf° = -689.946 - 76.052x10⁻³TlnT + 14.312x10⁻⁶T² + 2513.075T⁻¹ + 882.821x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15	136.309	140.498	140.498	0	-668.620	-555.894	407.476
300	136.389	141.342	140.502	.252	-668.541	-555.195	404.454
400	139.409	180.993	145.885	14.043	-664.081	-518.079	283.062
500	142.419	212.425	156.157	28.134	-659.484	-482.109	210.727
600	145.429	238.657	167.780	42.526	-654.730	-447.079	162.846
700	148.439	261.301	179.558	57.220	-649.816	-412.856	128.898
800	151.450	281.319	191.051	72.214	-644.742	-379.352	103.633
900	154.460	299.331	202.098	87.510	-639.492	-346.492	84.139
1000	157.470	315.761	212.655	103.106	-634.066	-314.231	68.674

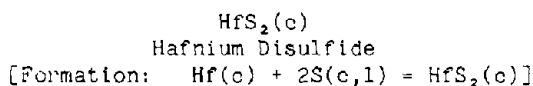
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $\text{Cp}^\circ = 127.506 + 29.940 \times 10^{-3}T - 0.110 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 127.506 \times 10^{-3}T + 14.970 \times 10^{-6}T^2 + 0.110 \times 10^{-2}T^{-1} - 39.384$

Reaction equations (kcal/mol):

298.15-1000 K: $\Delta H_r^\circ = -679.983 + 36.957 \times 10^{-3}T + 9.027 \times 10^{-6}T^2 - 136.700T^{-1}$
 $\Delta G_r^\circ = -679.983 - 36.957 \times 10^{-3}T \ln T - 9.027 \times 10^{-6}T^2 - 68.350T^{-1} + 630.221 \times 10^{-3}T$

Source: Data from Chase (17).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15*	16.210	20.000	20.000	0	-140.000	-138.291	101.369
300	16.230	20.100	20.000	.030	-140.001	-138.279	100.735
368.3	16.715	23.481	20.340	1.157	-140.067	-137.883	81.819
368.3	16.715	23.481	20.340	1.157	-140.259	-137.883	81.819
388.36	16.857	24.371	20.526	1.493	-140.287	-137.752	77.519
388.36	16.857	24.371	20.526	1.493	-141.113	-137.752	77.519
400	16.940	24.870	20.645	1.690	-141.166	-137.651	75.208
432.02	17.113	26.181	21.007	2.235	-141.351	-137.364	69.488
500	17.480	28.710	21.890	3.410	-141.962	-136.680	59.742
600	17.940	31.940	23.307	5.180	-142.567	-135.569	49.380
700	18.360	34.740	24.740	7.000	-143.026	-134.359	41.948
717.824	18.433	35.202	24.994	7.328	-143.095	-134.136	40.839

*Enthalpy of formation and entropy at 298 K estimated.

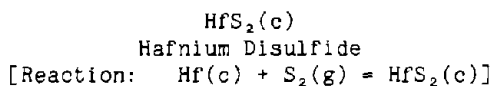
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1800 K: Cp° = 15.887 + 3.740x10⁻³T - 0.704x10⁻⁵T²
H° - H₂₉₈° = 15.887x10⁻³T + 1.870x10⁻⁶T² + 0.704x10⁻²T³ - 5.139

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -137.773 - 6.070x10⁻³T + 4.394x10⁻⁶T² - 240.800T⁻¹
ΔGf° = -137.773 + 6.070x10⁻³T ln T - 4.394x10⁻⁶T² - 120.400T⁻¹ - 33.657x10⁻³T
368.3-388.36 K: ΔHf° = -140.003 - 1.544x10⁻³T + 0.902x10⁻⁶T² + 70.400T⁻¹
ΔGf° = -140.003 + 1.544x10⁻³T ln T - 0.902x10⁻⁶T² + 35.200T⁻¹ - 3.291x10⁻³T
388.36-432.02 K: ΔHf° = -172.320 + 87.936x10⁻³T - 85.662x10⁻⁶T² + 3874.800T⁻¹
ΔGf° = -172.320 - 87.936x10⁻³T ln T + 85.662x10⁻⁶T² + 1937.400T⁻¹ + 567.166x10⁻³T
432.02-717.824 K: ΔHf° = -191.277 + 80.124x10⁻³T - 46.038x10⁻⁶T² + 10327.800T⁻¹
ΔGf° = -191.277 - 80.124x10⁻³T ln T + 46.038x10⁻⁶T² + 5163.900T⁻¹ + 563.471x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	16.210	20	20	0	-170.710	-157.318	115.316
300	16.230	20.100	20	.030	-170.705	-157.234	114.543
400	16.940	24.870	20.645	1.690	-170.468	-152.782	83.475
500	17.480	28.710	21.890	3.410	-170.217	-148.386	64.859
600	17.940	31.940	23.307	5.180	-169.956	-144.050	52.470
700	18.360	34.740	24.740	7.000	-169.676	-139.749	43.631
800	18.770	37.220	26.145	8.860	-169.385	-135.491	37.014
900	19.170	39.450	27.506	10.750	-169.090	-131.279	31.879
1000	19.560	41.490	28.800	12.690	-168.771	-127.094	27.776
1100	19.940	43.370	30.043	14.660	-168.448	-122.941	24.426
1200	20.330	45.120	31.220	16.680	-168.100	-118.810	21.638
1300	20.710	46.770	32.362	18.730	-167.748	-114.731	19.288
1400	21.090	48.310	33.439	20.820	-167.381	-110.650	17.273
1500	21.470	49.780	34.480	22.950	-167.000	-106.611	15.533
1600	21.840	51.180	35.486	25.110	-166.614	-102.614	14.016
1700	22.220	52.520	36.455	27.310	-166.215	-98.642	12.681
1800	22.600	53.800	37.378	29.560	-165.788	-94.654	11.492

*Enthalpy of formation and entropy at 298 K estimated.

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

298.15-1800 K: $C_p^\circ = 15.887 + 3.740 \times 10^{-3}T - 0.704 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 15.887 \times 10^{-3}T + 1.870 \times 10^{-6}T^2 + 0.704 \times 10^{-2}T^{-1} - 5.139$

Reaction equations (kcal/mol):

298.15-1800 K: $\Delta H_r^\circ = -171.351 + 1.935 \times 10^{-3}T + 0.640 \times 10^{-6}T^2 + 2.100T^{-1}$
 $\Delta G_r^\circ = -171.351 - 1.935 \times 10^{-3}T \ln T - 0.640 \times 10^{-6}T^2 + 1.050T^{-1} + 58.269 \times 10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K are those estimated by Mills (80). Other data based on Volovik (125).

HgS(red, black)
Mercury Sulfide
[Formation: $\text{Hg(l,g)} + \text{S(c,l)} = \text{HgS(c)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	11.570	19.720	19.720	0	-13.000	-11.187	8.200
300*	11.580	19.790	19.720	.021	-13.001	-11.175	8.141
350	11.920	21.600	19.860	.609	-13.024	-10.868	6.786
368.3	12.026	22.210	19.962	.828	-13.031	-10.756	6.382
368.3	12.026	22.210	19.962	.828	-13.127	-10.756	6.382
388.36	12.142	22.850	20.092	1.071	-13.134	-10.624	5.979
388.36	12.142	22.850	20.092	1.071	-13.547	-10.624	5.979
400	12.210	23.210	20.177	1.213	-13.570	-10.537	5.757
432.02	12.377	24.163	20.445	1.607	-13.649	-10.294	5.208
450	12.470	24.670	20.603	1.830	-13.765	-10.153	4.931
500	12.700	25.990	21.070	2.460	-13.912	-9.739	4.257
550	12.910	27.210	21.574	3.100	-14.033	-9.316	3.702
600	13.110	28.350	22.100	3.750	-14.128	-8.888	3.237
618	13.170	28.740	22.289	3.987	-14.154	-8.729	3.087
618	13.170	30.360	22.289	4.987	-13.154	-8.729	3.087
629.81	13.214	30.610	22.444	5.143	-13.171	-8.646	3.000
629.81	13.214	30.610	22.444	5.143	-27.322	-8.646	3.000
650	13.290	31.020	22.697	5.410	-27.317	-8.042	2.704
700	13.480	32.010	23.324	6.080	-27.290	-6.557	2.047
717.824	13.544	32.350	23.544	6.321	-27.275	-6.029	1.836

*Data above 298 K estimated except temperature and enthalpy of transition.

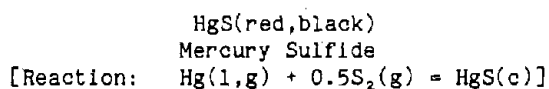
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
618 K, red - black transition point of HgS; $\Delta H^\circ = 1.000$ kcal/mol.
629.81 K, boiling point of Hg; $\Delta H^\circ = 14.151$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-618 K: $C_p^\circ = 11.048 + 3.710 \times 10^{-3}T - 0.519 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 11.048 \times 10^{-3}T + 1.855 \times 10^{-6}T^2 + 0.519 \times 10^{-2}T^3 - 3.633$
 618-900 K: $C_p^\circ = 11.761 + 2.856 \times 10^{-3}T - 1.360 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 11.761 \times 10^{-3}T + 1.428 \times 10^{-6}T^2 + 1.360 \times 10^{-2}T^3 - 3.047$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -12.053 - 3.399 \times 10^{-3}T + 3.471 \times 10^{-6}T^2 - 72.300T^{-1}$
 $\Delta G_f^\circ = -12.053 + 3.399 \times 10^{-3}T \ln T - 3.471 \times 10^{-6}T^2 - 36.150T^{-1} - 15.021 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -13.168 - 1.136 \times 10^{-3}T + 1.725 \times 10^{-6}T^2 + 83.300T^{-1}$
 $\Delta G_f^\circ = -13.168 + 1.136 \times 10^{-3}T \ln T - 1.725 \times 10^{-6}T^2 + 41.650T^{-1} + 0.162 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -29.326 + 43.604 \times 10^{-3}T - 41.557 \times 10^{-6}T^2 + 1985.500T^{-1}$
 $\Delta G_f^\circ = -29.326 - 43.604 \times 10^{-3}T \ln T + 41.557 \times 10^{-6}T^2 + 992.750T^{-1} + 285.390 \times 10^{-3}T$
 432.02-618 K: $\Delta H_f^\circ = -38.805 + 39.698 \times 10^{-3}T - 21.745 \times 10^{-6}T^2 + 5212.000T^{-1}$
 $\Delta G_f^\circ = -38.805 - 39.698 \times 10^{-3}T \ln T + 21.745 \times 10^{-6}T^2 + 2606.000T^{-1} + 283.543 \times 10^{-3}T$
 618-629.81 K: $\Delta H_f^\circ = -38.218 + 40.411 \times 10^{-3}T - 22.172 \times 10^{-6}T^2 + 5296.100T^{-1}$
 $\Delta G_f^\circ = -38.218 - 40.411 \times 10^{-3}T \ln T + 22.172 \times 10^{-6}T^2 + 2648.050T^{-1} + 286.802 \times 10^{-3}T$
 629.81-717.824 K: $\Delta H_f^\circ = -53.181 + 41.716 \times 10^{-3}T - 22.071 \times 10^{-6}T^2 + 5264.700T^{-1}$
 $\Delta G_f^\circ = -53.181 - 41.716 \times 10^{-3}T \ln T + 22.071 \times 10^{-6}T^2 + 2632.350T^{-1} + 319.075 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	11.570	19.720	19.720	0	-28.355	-20.701	15.174
300*	11.580	19.790	19.720	.021	-28.353	-20.652	15.045
350	11.920	21.600	19.860	.609	-28.294	-19.373	12.097
400	12.210	23.210	20.177	1.213	-28.221	-18.102	9.891
450	12.470	24.670	20.603	1.830	-28.136	-16.845	8.181
500	12.700	25.990	21.070	2.460	-28.040	-15.592	6.815
550	12.910	27.210	21.574	3.100	-27.935	-14.354	5.703
600	13.110	28.350	22.100	3.750	-27.823	-13.129	4.782
618	13.170	28.740	22.289	3.987	-27.779	-12.688	4.487
618	13.170	30.360	22.289	4.987	-26.779	-12.688	4.487
629.81	13.214	30.610	22.444	5.143	-26.750	-12.420	4.310
629.81	13.214	30.610	22.444	5.143	-40.901	-12.420	4.310
650	13.290	31.020	22.697	5.410	-40.821	-11.503	3.868
700	13.480	32.010	23.324	6.080	-40.615	-9.253	2.889
750	13.660	32.950	23.939	6.758	-40.403	-7.023	2.047
800	13.830	33.840	24.533	7.446	-40.182	-4.807	1.313
850	14.000	34.680	25.101	8.142	-39.954	-2.600	.668
900	14.170	35.490	25.661	8.846	-39.718	-1.414	.100

*Data above 298 K estimated except temperature and enthalpy of transition.

Phase changes: 618 K, red - black transition point of HgS; ΔH° = 1.000 kcal/mol.
629.81 K, boiling point of Hg; ΔH° = 14.151 kcal/mol.

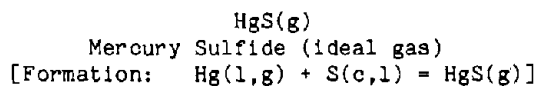
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-618 K: $\text{Cp}^\circ = 11.048 + 3.710 \times 10^{-3}T - 0.519 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 11.048 \times 10^{-3}T + 1.855 \times 10^{-6}T^2 + 0.519 \times 10^{-2}T^{-1} - 3.633$
 618-900 K: $\text{Cp}^\circ = 11.761 + 2.856 \times 10^{-3}T - 1.360 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 11.761 \times 10^{-3}T + 1.428 \times 10^{-6}T^2 + 1.360 \times 10^{-2}T^{-1} - 3.047$

Reaction equations (kcal/mol):

298.15-618 K: $\Delta\text{Hr}^\circ = -28.841 + 0.604 \times 10^{-3}T + 1.594 \times 10^{-6}T^2 + 49.150T^{-1}$
 $\Delta\text{Gr}^\circ = -28.841 - 0.604 \times 10^{-3}T \ln T - 1.594 \times 10^{-6}T^2 + 24.575T^{-1} + 30.942 \times 10^{-3}T$
 618-629.81 K: $\Delta\text{Hr}^\circ = -28.255 + 1.316 \times 10^{-3}T + 1.167 \times 10^{-6}T^2 + 133.250T^{-1}$
 $\Delta\text{Gr}^\circ = -28.255 - 1.316 \times 10^{-3}T \ln T - 1.167 \times 10^{-6}T^2 + 66.625T^{-1} + 34.201 \times 10^{-3}T$
 629.81-900 K: $\Delta\text{Hr}^\circ = -43.218 + 2.621 \times 10^{-3}T + 1.268 \times 10^{-6}T^2 + 101.850T^{-1}$
 $\Delta\text{Gr}^\circ = -43.218 - 2.621 \times 10^{-3}T \ln T - 1.268 \times 10^{-6}T^2 + 50.925T^{-1} + 66.474 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Goldfinger (45), Mitchell (82), Treadwell (119), and Grade (46). Low-temperature heat capacities and entropy at 298 K from King (67). High-temperature data estimated except temperature and enthalpy of transition.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	8.675	60.745	60.745	0	32.000	21.581	-15.819
300	8.679	60.799	60.746	.016	31.994	21.517	-15.675
368.3	8.776	62.591	60.926	.613	31.754	19.157	-11.368
368.3	8.776	62.591	60.926	.613	31.658	19.157	-11.368
388.36	8.804	63.057	61.024	.789	31.584	18.479	-10.399
388.36	8.804	63.057	61.024	.789	31.171	18.479	-10.399
400	8.821	63.317	61.087	.892	31.109	18.099	-9.889
432.02	8.846	63.997	61.278	1.175	30.919	17.065	-8.633
500	8.899	65.295	61.739	1.778	30.406	14.927	-6.524
600	8.950	66.922	62.470	2.671	29.793	11.890	-4.331
629.81	8.961	67.356	62.691	2.938	29.624	11.006	-3.819
629.81	8.961	67.356	62.691	2.938	15.473	11.006	-3.819
700	8.987	68.304	63.207	3.568	15.198	10.525	-3.286
717.824	8.992	68.530	63.336	3.728	15.133	10.407	-3.169

*Data except enthalpy of formation at 298 K estimated.

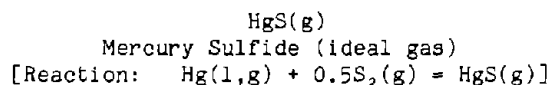
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 629.81 K, boiling point of Hg; $\Delta H^\circ = 14.151$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-3000 K: $C_p^\circ = 8.929 + 0.158 \times 10^{-3}T - 0.268 \times 10^{-5}T^2$
 $H^\circ - H^\circ_{298} = 8.929 \times 10^{-3}T + 0.079 \times 10^{-6}T^2 + 0.268 \times 10^{-2}T^{-1} - 2.759$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 33.821 - 5.518 \times 10^{-3}T + 1.695 \times 10^{-6}T^2 - 97.400T^{-1}$
 $\Delta G_f^\circ = 33.821 + 5.518 \times 10^{-3}T \ln T - 1.695 \times 10^{-6}T^2 - 48.700T^{-1} - 71.438 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = 32.706 - 3.255 \times 10^{-3}T - 0.051 \times 10^{-6}T^2 + 58.200T^{-1}$
 $\Delta G_f^\circ = 32.706 + 3.255 \times 10^{-3}T \ln T + 0.051 \times 10^{-6}T^2 + 29.100T^{-1} - 56.256 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = 16.548 + 41.485 \times 10^{-3}T - 43.333 \times 10^{-6}T^2 + 1960.400T^{-1}$
 $\Delta G_f^\circ = 16.548 - 41.485 \times 10^{-3}T \ln T + 43.333 \times 10^{-6}T^2 + 980.200T^{-1} + 228.973 \times 10^{-3}T$
 432.02-629.81 K: $\Delta H_f^\circ = 7.069 + 37.579 \times 10^{-3}T - 23.521 \times 10^{-6}T^2 + 5186.900T^{-1}$
 $\Delta G_f^\circ = 7.069 - 37.579 \times 10^{-3}T \ln T + 23.521 \times 10^{-6}T^2 + 2593.450T^{-1} + 227.125 \times 10^{-3}T$
 629.81-717.824 K: $\Delta H_f^\circ = -7.894 + 38.884 \times 10^{-3}T - 23.420 \times 10^{-6}T^2 + 5155.500T^{-1}$
 $\Delta G_f^\circ = -7.894 - 38.884 \times 10^{-3}T \ln T + 23.420 \times 10^{-6}T^2 + 2577.750T^{-1} + 259.398 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	8.675	60.745	60.745	0	16.645	12.068	-8.846
300	8.679	60.799	60.746	.016	16.642	12.040	-8.771
400	8.821	63.317	61.087	.892	16.458	10.534	-5.755
500	8.899	65.295	61.739	1.778	16.278	9.073	-3.966
600	8.950	66.922	62.470	2.671	16.099	7.649	-2.786
629.81	8.961	67.356	62.691	2.938	16.045	7.232	-2.510
629.81	8.961	67.356	62.691	2.938	1.894	7.232	-2.510
700	8.987	68.304	63.207	3.568	1.873	7.830	-2.444
800	9.016	69.506	63.921	4.468	1.840	8.683	-2.372
900	9.041	70.570	64.602	5.371	1.806	9.539	-2.316
1000	9.063	71.524	65.248	6.276	1.771	10.400	-2.273
1100	9.084	72.388	65.858	7.183	1.733	11.264	-2.238
1200	9.103	73.180	66.436	8.093	1.696	12.133	-2.210
1300	9.121	73.909	66.983	9.004	1.656	13.004	-2.186
1400	9.139	74.586	67.502	9.917	1.613	13.879	-2.167
1500	9.156	75.217	67.996	10.832	1.569	14.755	-2.150
1600	9.173	75.808	68.465	11.748	1.523	15.637	-2.136
1700	9.189	76.365	68.914	12.666	1.474	16.519	-2.124
1800	9.205	76.890	69.342	13.586	1.427	17.408	-2.114
1900	9.222	77.388	69.753	14.507	1.375	18.297	-2.105
2000	9.238	77.862	70.147	15.430	1.322	19.189	-2.097

*Data except enthalpy of formation at 298 K estimated.

Phase change: 629.81 K, boiling point of Hg; ΔH° = 14.151 kcal/mol.

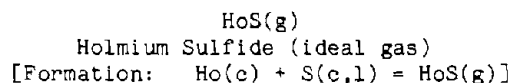
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $C_p^\circ = 8.929 + 0.158 \times 10^{-3}T - 0.268 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 8.929 \times 10^{-3}T + 0.079 \times 10^{-6}T^2 + 0.268 \times 10^{-2}T^{-1} - 2.759$

Reaction equations (kcal/mol):

298.15-629.81 K: $\Delta H_r^\circ = 17.032 - 1.515 \times 10^{-3}T - 0.182 \times 10^{-6}T^2 + 24.050T^{-1}$
 $\Delta G_r^\circ = 17.032 + 1.515 \times 10^{-3}T \ln T + 0.182 \times 10^{-6}T^2 + 12.025T^{-1} - 25.475 \times 10^{-3}T$
629.81-2000 K: $\Delta H_r^\circ = 2.069 - 0.211 \times 10^{-3}T - 0.081 \times 10^{-6}T^2 - 7.350T^{-1}$
 $\Delta G_r^\circ = 2.069 + 0.211 \times 10^{-3}T \ln T + 0.081 \times 10^{-6}T^2 - 3.675T^{-1} + 6.797 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Goldfinger (45). Other data estimated.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	8.200	63.920	63.920	0	35.400	23.972	-17.572
300	8.210	63.970	63.920	.015	35.393	23.902	-17.412
368.3	8.415	65.681	64.094	.585	35.131	21.311	-12.646
368.3	8.415	65.681	64.094	.585	35.035	21.311	-12.646
388.36	8.475	66.129	64.187	.754	34.952	20.567	-11.574
388.36	8.475	66.129	64.187	.754	34.539	20.567	-11.574
400	8.510	66.380	64.247	.853	34.473	20.149	-11.009
432.02	8.555	67.037	64.430	1.126	34.270	19.009	-9.616
500	8.650	68.290	64.866	1.712	33.725	16.659	-7.281
600	8.730	69.880	65.578	2.581	33.061	13.304	-4.846
700	8.780	71.230	66.293	3.456	32.461	10.058	-3.140
717.824	8.785	71.451	66.418	3.613	32.359	9.490	-2.889

*Data except enthalpy of formation at 298 K estimated.

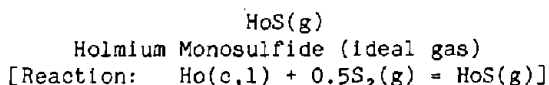
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: $C_p^\circ = 8.875 + 0.036 \times 10^{-3} T - 0.608 \times 10^{-5} T^2$
 $H^\circ - H_{298}^\circ = 8.875 \times 10^{-3} T + 0.018 \times 10^{-6} T^2 + 0.608 \times 10^{-2} T^{-1} - 2.852$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 36.032 - 2.640 \times 10^{-3} T - 0.590 \times 10^{-6} T^2 + 61.900 T^{-1}$
 $\Delta G_f^\circ = 36.032 + 2.640 \times 10^{-3} T \ln T + 0.590 \times 10^{-6} T^2 + 30.950 T^{-1} - 56.014 \times 10^{-3} T$
368.3-388.36 K: $\Delta H_f^\circ = 34.917 - 0.377 \times 10^{-3} T - 2.336 \times 10^{-6} T^2 + 217.500 T^{-1}$
 $\Delta G_f^\circ = 34.917 + 0.377 \times 10^{-3} T \ln T + 2.336 \times 10^{-6} T^2 + 108.750 T^{-1} - 40.831 \times 10^{-3} T$
388.36-432.02 K: $\Delta H_f^\circ = 18.759 + 44.363 \times 10^{-3} T - 45.618 \times 10^{-6} T^2 + 2119.700 T^{-1}$
 $\Delta G_f^\circ = 18.759 - 44.363 \times 10^{-3} T \ln T + 45.618 \times 10^{-6} T^2 + 1059.850 T^{-1} + 244.397 \times 10^{-3} T$
432.02-717.824 K: $\Delta H_f^\circ = 9.280 + 40.457 \times 10^{-3} T - 25.806 \times 10^{-6} T^2 + 5346.200 T^{-1}$
 $\Delta G_f^\circ = 9.280 - 40.457 \times 10^{-3} T \ln T + 25.806 \times 10^{-6} T^2 + 2673.100 T^{-1} + 242.550 \times 10^{-3} T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15*	8.200	63.920	63.920	0	20.045	14.459	-10.598
300	8.210	63.970	63.920	.015	20.041	14.424	-10.508
400	8.510	66.380	64.247	.853	19.822	12.583	-6.875
500	8.650	68.290	64.866	1.712	19.598	10.805	-4.723
600	8.730	69.880	65.578	2.581	19.367	9.063	-3.301
700	8.780	71.230	66.293	3.456	19.136	7.363	-2.299
800	8.810	72.400	66.980	4.336	18.893	5.704	-1.558
900	8.830	73.440	67.642	5.218	18.625	4.072	-.989
1000	8.850	74.370	68.268	6.102	18.322	2.471	-.540
1100	8.860	75.220	68.867	6.988	17.978	.889	-.177
1200	8.880	75.990	69.427	7.875	17.582	-.637	.116
1300	8.890	76.700	69.959	8.763	17.126	-2.139	.360
1400	8.890	77.360	70.466	9.652	16.602	-3.599	.562
1500	8.900	77.970	70.942	10.542	16.002	-5.014	.731
1600	8.910	78.550	71.405	11.432	15.316	-6.412	.876
1700	8.910	79.090	71.841	12.323	14.539	-7.741	.995
1701	8.910	79.095	71.845	12.332	14.530	-7.766	.998
1701	8.910	79.095	71.845	12.332	13.409	-7.766	.998
1743	8.914	79.313	72.023	12.706	13.304	-8.275	1.038
1743	8.914	79.313	72.023	12.706	10.393	-8.275	1.038
1800	8.920	79.600	72.258	13.215	10.034	-8.876	1.078
1900	8.930	80.080	72.655	14.108	9.401	-9.919	1.141
2000	8.930	80.540	73.040	15.000	8.764	-10.921	1.193

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 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:

298.15-2000 K: $C_p^\circ = 8.875 + 0.036 \times 10^{-3}T - 0.608 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 8.875 \times 10^{-3}T + 0.018 \times 10^{-6}T^2 + 0.608 \times 10^2 T^{-1} - 2.852$

Reaction equations (kcal/mol):

298.15-1701 K: $\Delta H_r^\circ = 19.243 + 1.363 \times 10^{-3}T - 2.467 \times 10^{-6}T^2 + 183.350T^{-1}$
 $\Delta G_r^\circ = 19.243 - 1.363 \times 10^{-3}T \ln T + 2.467 \times 10^{-6}T^2 + 91.675T^{-1} - 10.051 \times 10^{-3}T$
1701-1743 K: $\Delta H_r^\circ = 17.201 - 1.996 \times 10^{-3}T - 0.142 \times 10^{-6}T^2 + 26.650T^{-1}$
 $\Delta G_r^\circ = 17.201 + 1.996 \times 10^{-3}T \ln T + 0.142 \times 10^{-6}T^2 + 13.325T^{-1} - 29.856 \times 10^{-3}T$
1743-2000 K: $\Delta H_r^\circ = 20.913 - 5.796 \times 10^{-3}T - 0.142 \times 10^{-6}T^2 + 26.650T^{-1}$
 $\Delta G_r^\circ = 20.913 + 5.796 \times 10^{-3}T \ln T + 0.142 \times 10^{-6}T^2 + 13.325T^{-1} - 60.347 \times 10^{-3}T$

Source: Data from Mills (80) who estimated all except enthalpy of formation at 298 K.

InS(c)
Indium Monosulfide
[Formation: $\text{In(c,l)} + \text{S(c,l)} = \text{InS(c)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	11.500	16.960	16.960	0	-32.000	-30.652	22.468
300*	11.510	17.030	16.960	.021	-32.001	-30.643	22.323
368.3	12.022	19.448	17.199	.828	-32.025	-30.332	17.999
368.3	12.022	19.448	17.199	.828	-32.121	-30.332	17.999
388.36	12.173	20.089	17.332	1.071	-32.134	-30.234	17.014
388.36	12.173	20.089	17.332	1.071	-32.547	-30.234	17.014
400	12.260	20.450	17.418	1.213	-32.573	-30.164	16.481
429.78	12.424	21.336	17.659	1.581	-32.650	-29.982	15.246
429.78	12.424	21.336	17.659	1.581	-33.430	-29.982	15.246
432.02	12.436	21.401	17.678	1.608	-33.446	-29.964	15.158
500	12.810	23.250	18.316	2.467	-33.740	-29.392	12.847
600	13.240	25.630	19.345	3.771	-33.995	-28.498	10.380
700	13.620	27.700	20.394	5.114	-34.152	-27.569	8.607
717.824	13.681	28.043	20.580	5.357	-34.170	-27.400	8.342

*Data above 298 K estimated.

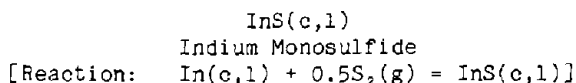
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 429.78 K, melting point of In; $\Delta H^\circ = 0.780$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-965 K: $\text{Cp}^\circ = 11.613 + 3.112 \times 10^{-3}T - 0.925 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 11.613 \times 10^{-3}T + 1.556 \times 10^{-6}T^2 + 0.925 \times 10^{-2}T^{-1} - 3.911$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta \text{Hf}^\circ = -32.178 + 0.819 \times 10^{-3}T - 1.489 \times 10^{-6}T^2 + 19.600T^{-1}$
 $\Delta \text{Gf}^\circ = -32.178 - 0.819 \times 10^{-3}T \ln T + 1.489 \times 10^{-6}T^2 + 9.800T^{-1} + 9.229 \times 10^{-3}T$
 368.3-388.36 K: $\Delta \text{Hf}^\circ = -33.293 + 3.082 \times 10^{-3}T - 3.235 \times 10^{-6}T^2 + 175.200T^{-1}$
 $\Delta \text{Gf}^\circ = -33.293 - 3.082 \times 10^{-3}T \ln T + 3.235 \times 10^{-6}T^2 + 87.600T^{-1} + 24.412 \times 10^{-3}T$
 388.36-429.78 K: $\Delta \text{Hf}^\circ = -49.451 + 47.822 \times 10^{-3}T - 46.517 \times 10^{-6}T^2 + 2077.400T^{-1}$
 $\Delta \text{Gf}^\circ = -49.451 - 47.822 \times 10^{-3}T \ln T + 46.517 \times 10^{-6}T^2 + 1038.700T^{-1} + 309.640 \times 10^{-3}T$
 429.78-432.02 K: $\Delta \text{Hf}^\circ = -49.091 + 43.475 \times 10^{-3}T - 41.745 \times 10^{-6}T^2 + 2011.700T^{-1}$
 $\Delta \text{Gf}^\circ = -49.091 - 43.475 \times 10^{-3}T \ln T + 41.745 \times 10^{-6}T^2 + 1005.850T^{-1} + 284.675 \times 10^{-3}T$
 432.02-717.824 K: $\Delta \text{Hf}^\circ = -58.570 + 39.569 \times 10^{-3}T - 21.933 \times 10^{-6}T^2 + 5238.200T^{-1}$
 $\Delta \text{Gf}^\circ = -58.570 - 39.569 \times 10^{-3}T \ln T + 21.933 \times 10^{-6}T^2 + 2619.100T^{-1} + 282.827 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	11.500	16.960	16.960	0	-47.355	-40.166	29.442
300*	11.510	17.030	16.960	.021	-47.353	-40.121	29.228
400	12.260	20.450	17.418	1.213	-47.224	-37.730	20.614
429.78	12.424	21.336	17.659	1.581	-47.188	-37.024	18.827
429.78	12.424	21.336	17.659	1.581	-47.968	-37.024	18.827
500	12.810	23.250	18.316	2.467	-47.868	-35.245	15.405
600	13.240	25.630	19.345	3.771	-47.689	-32.739	11.925
700	13.620	27.700	20.394	5.114	-47.477	-30.264	9.449
800	13.960	29.540	21.423	6.494	-47.231	-27.819	7.600
900	14.270	31.200	22.416	7.906	-46.954	-25.407	6.170
965	14.470	32.200	23.038	8.840	-46.760	-23.854	5.402
965	14.500	41.110	23.038	17.440	-38.160	-23.854	5.402
1000	14.500	41.630	23.682	17.948	-38.051	-23.340	5.101
1100	14.500	43.010	25.375	19.398	-37.743	-21.880	4.347
1200	14.500	44.270	26.897	20.848	-37.440	-20.451	3.724
1300	14.500	45.440	28.288	22.298	-37.139	-19.060	3.204
1400	14.500	46.510	29.547	23.748	-36.843	-17.672	2.759

*Data above 298 K estimated.

Phase changes: 429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.
965 K, melting point of InS; ΔH° = 8.600 kcal/mol.

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

298.15-965 K: $C_p^\circ = 11.613 + 3.112 \times 10^{-3}T - 0.925 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 11.613 \times 10^{-3}T + 1.556 \times 10^{-6}T^2 + 0.925 \times 10^{-2}T^{-1} - 3.911$
 965-1400 K: $C_p^\circ = 14.500$
 $H^\circ - H_{298}^\circ = 14.500 \times 10^{-3}T + 3.448$

Reaction equations (kcal/mol):

298.15-429.78 K: $\Delta H_r^\circ = -48.966 + 4.822 \times 10^{-3}T - 3.366 \times 10^{-6}T^2 + 141.050T^{-1}$
 $\Delta G_r^\circ = -48.966 - 4.822 \times 10^{-3}T \ln T + 3.366 \times 10^{-6}T^2 + 70.525T^{-1} + 55.192 \times 10^{-3}T$
 429.78-965 K: $\Delta H_r^\circ = -48.607 + 0.474 \times 10^{-3}T + 1.406 \times 10^{-6}T^2 + 75.350T^{-1}$
 $\Delta G_r^\circ = -48.607 - 0.474 \times 10^{-3}T \ln T - 1.406 \times 10^{-6}T^2 + 37.675T^{-1} + 30.227 \times 10^{-3}T$
 965-1400 K: $\Delta H_r^\circ = -41.248 + 3.361 \times 10^{-3}T - 0.150 \times 10^{-6}T^2 - 17.150T^{-1}$
 $\Delta G_r^\circ = -41.248 - 3.361 \times 10^{-3}T \ln T + 0.150 \times 10^{-6}T^2 - 8.575T^{-1} + 40.989 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mills (80). Low-temperature heat capacities and entropy at 298 K from Mamedov (76). High-temperature data estimated. Estimates of fusion data and heat capacity of liquid from Mills.

InS(g)
Indium Monosulfide (ideal gas)
[Formation: In(c,l) + S(c,l) = InS(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15*	8.380	60.150	60.150	0	55.700	44.171	-32.378
300	8.390	60.200	60.150	.015	55.693	44.100	-32.126
368.3	8.547	61.951	60.333	.596	55.443	41.482	-24.615
368.3	8.547	61.951	60.333	.596	55.347	41.482	-24.615
388.36	8.593	62.406	60.429	.768	55.263	40.729	-22.920
388.36	8.593	62.406	60.429	.768	54.850	40.729	-22.920
400	8.620	62.660	60.490	.868	54.782	40.307	-22.022
429.78	8.653	63.280	60.662	1.125	54.595	39.236	-19.952
429.78	8.653	63.280	60.662	1.125	53.815	39.236	-19.952
432.02	8.655	63.325	60.676	1.145	53.790	39.160	-19.810
500	8.730	64.590	61.118	1.736	53.229	36.908	-16.132
600	8.790	66.190	61.837	2.612	52.546	33.707	-12.278
700	8.820	67.540	62.551	3.492	51.926	30.622	-9.560
717.824	8.825	67.762	62.678	3.649	51.822	30.081	-9.158

*Data except enthalpy of formation at 298 K estimated.

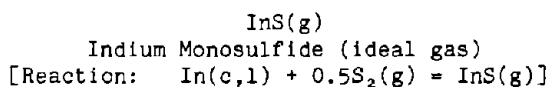
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 8.905 + 0.020x10⁻³T - 0.472x10⁻⁵T⁻²
H° - H₂₉₈° = 8.905x10⁻³T + 0.010x10⁻⁶T² + 0.472x10⁻²T⁻¹ - 2.814

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 56.619 - 1.889x10⁻³T - 3.035x10⁻⁶T² - 25.700T⁻¹
ΔGf° = 56.619 + 1.889x10⁻³TlnT + 3.035x10⁻⁶T² - 12.850T⁻¹ - 53.275x10⁻³T
368.3-388.36 K: ΔHf° = 55.504 + 0.374x10⁻³T - 4.781x10⁻⁶T² + 129.900T⁻¹
ΔGf° = 55.504 - 0.374x10⁻³TlnT + 4.781x10⁻⁶T² + 64.950T⁻¹ - 38.092x10⁻³T
388.36-429.78 K: ΔHf° = 39.346 + 45.114x10⁻³T - 48.063x10⁻⁶T² + 2032.100T⁻¹
ΔGf° = 39.346 - 45.114x10⁻³TlnT + 48.063x10⁻⁶T² + 1016.050T⁻¹ + 247.136x10⁻³T
429.78-432.02 K: ΔHf° = 39.705 + 40.767x10⁻³T - 43.291x10⁻⁶T² + 1966.400T⁻¹
ΔGf° = 39.705 - 40.767x10⁻³TlnT + 43.291x10⁻⁶T² + 983.200T⁻¹ + 222.171x10⁻³T
432.02-717.824 K: ΔHf° = 30.227 + 36.861x10⁻³T - 23.479x10⁻⁶T² + 5192.900T⁻¹
ΔGf° = 30.227 - 36.861x10⁻³TlnT + 23.479x10⁻⁶T² + 2596.450T⁻¹ + 220.324x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15*	8.380	60.150	60.150	0	40.345	34.657	-25.404
300	8.390	60.200	60.150	.015	40.341	34.622	-25.222
400	8.620	62.660	60.490	.868	40.131	32.741	-17.889
429.78	8.653	63.280	60.662	1.125	40.056	32.194	-16.371
429.78	8.653	63.280	60.662	1.125	39.276	32.194	-16.371
500	8.730	64.590	61.118	1.736	39.102	31.054	-13.574
600	8.790	66.190	61.837	2.612	38.852	29.466	-10.733
700	8.820	67.540	62.551	3.492	38.601	27.926	-8.719
800	8.850	68.720	63.250	4.376	38.352	26.419	-7.217
900	8.860	69.770	63.924	5.261	38.101	24.935	-6.055
1000	8.880	70.700	64.551	6.149	37.850	23.492	-5.134
1100	8.890	71.550	65.153	7.037	37.596	22.065	-4.384
1200	8.900	72.320	65.715	7.926	37.339	20.668	-3.764
1300	8.900	73.040	66.258	8.816	37.079	19.278	-3.241
1400	8.910	73.700	66.766	9.707	36.816	17.921	-2.798
1500	8.910	74.310	67.245	10.598	36.551	16.588	-2.417
1600	8.920	74.890	67.709	11.489	36.281	15.257	-2.084
1700	8.920	75.430	68.147	12.381	36.009	13.954	-1.794
1800	8.930	75.940	68.566	13.274	35.734	12.663	-1.537
1900	8.930	76.420	68.964	14.166	35.456	11.393	-1.311
2000	8.930	76.880	69.350	15.059	35.176	10.130	-1.107

*Data except enthalpy of formation at 298 K estimated.

Phase change: 429.78 K, melting point of In; $\Delta H^\circ = 0.780$ kcal/mol.

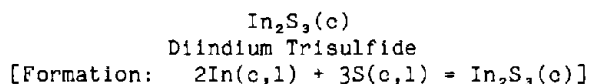
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 8.905 + 0.020 \times 10^{-3}T - 0.472 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 8.905 \times 10^{-3}T + 0.010 \times 10^{-6}T^2 + 0.472 \times 10^{-2}T^{-1} - 2.814$

Reaction equations (kcal/mol):

298.15-429.78 K: $\Delta H_r^\circ = 39.830 + 2.114 \times 10^{-3}T - 4.912 \times 10^{-6}T^2 + 95.750T^{-1}$
 $\Delta G_r^\circ = 39.830 - 2.114 \times 10^{-3}T \ln T + 4.912 \times 10^{-6}T^2 + 47.875T^{-1} - 7.312 \times 10^{-3}T$
 429.78-2000 K: $\Delta H_r^\circ = 40.190 - 2.234 \times 10^{-3}T - 0.140 \times 10^{-6}T^2 + 30.050T^{-1}$
 $\Delta G_r^\circ = 40.190 + 2.234 \times 10^{-3}T \ln T + 0.140 \times 10^{-6}T^2 + 15.025T^{-1} - 32.277 \times 10^{-3}T$

Source: Data from Mills (80) who estimated all except enthalpy of formation at 298 K.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	28.200	39.100	39.100	0	-85.000	-81.564	59.788
300	28.235	39.275	39.102	.052	-85.002	-81.543	59.403
368.3	29.119	45.178	39.695	2.019	-85.081	-80.751	47.917
368.3	29.119	45.178	39.695	2.019	-85.369	-80.751	47.917
388.36	29.378	46.729	40.018	2.606	-85.412	-80.496	45.299
388.36	29.378	46.729	40.018	2.606	-86.651	-80.496	45.299
400	29.529	47.599	40.226	2.949	-86.733	-80.311	43.880
429.78	29.729	49.727	40.812	3.831	-86.974	-79.825	40.592
429.78	29.729	49.727	40.812	3.831	-88.534	-79.825	40.592
432.02	29.744	49.881	40.859	3.898	-88.585	-79.779	40.358
500	30.200	54.267	42.391	5.938	-89.523	-78.311	34.229
600	30.630	59.813	44.845	8.981	-90.455	-75.975	27.674
660	30.828	62.742	46.340	10.825	-90.906	-74.505	24.671
660	32.060	63.151	46.340	11.095	-90.636	-74.505	24.671
700	32.600	65.054	47.357	12.388	-90.848	-73.522	22.954
717.824	32.841	65.877	47.806	12.971	-90.925	-73.078	22.249

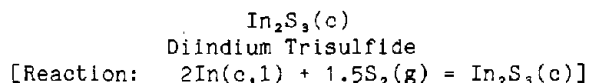
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 660 K, α - β transition point of In₂S₃; ΔH° = 0.270 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-660 K: Cp° = 30.434 + 1.416x10⁻³T - 2.356x10⁻⁵T²
 H° - H₂₉₈° = 30.434x10⁻³T + 0.708x10⁻⁶T² + 2.356x10⁻²T⁻¹ - 9.927
 660-1100 K: Cp° = 23.188 + 13.478x10⁻³T - 0.100x10⁻⁵T²
 H° - H₂₉₈° = 23.188x10⁻³T + 6.739x10⁻⁶T² + 0.100x10⁻²T⁻¹ - 7.160

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -84.654 + 0.672x10⁻³T - 3.665x10⁻⁶T² - 65.800T⁻¹
 ΔGf° = -84.654 - 0.672x10⁻³TlnT + 3.665x10⁻⁶T² - 32.900T⁻¹ + 13.468x10⁻³T
 368.3-388.36 K: ΔHf° = -87.999 + 7.461x10⁻³T - 8.903x10⁻⁶T² + 401.000T⁻¹
 ΔGf° = -87.999 - 7.461x10⁻³TlnT + 8.903x10⁻⁶T² + 200.500T⁻¹ + 59.017x10⁻³T
 388.36-429.78 K: ΔHf° = -136.474 + 141.681x10⁻³T - 138.749x10⁻⁶T² + 6107.600T⁻¹
 ΔGf° = -136.474 - 141.681x10⁻³TlnT + 138.749x10⁻⁶T² + 3053.800T⁻¹ + 914.702x10⁻³T
 429.78-432.02 K: ΔHf° = -135.755 + 132.987x10⁻³T - 129.205x10⁻⁶T² + 5976.200T⁻¹
 ΔGf° = -135.755 - 132.987x10⁻³TlnT + 129.205x10⁻⁶T² + 2988.100T⁻¹ + 864.772x10⁻³T
 432.02-660 K: ΔHf° = -164.191 + 121.269x10⁻³T - 69.769x10⁻⁶T² + 15655.700T⁻¹
 ΔGf° = -164.191 - 121.269x10⁻³TlnT + 69.769x10⁻⁶T² + 7827.850T⁻¹ + 859.229x10⁻³T
 660-717.824 K: ΔHf° = -161.424 + 114.023x10⁻³T - 63.738x10⁻⁶T² + 15430.100T⁻¹
 ΔGf° = -161.424 - 114.023x10⁻³TlnT + 63.738x10⁻⁶T² + 7715.050T⁻¹ + 812.233x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	28.200	39.100	39.100	0	-131.065	-110.105	80.708
300	28.235	39.275	39.102	.052	-131.058	-109.975	80.116
400	29.529	47.599	40.226	2.949	-130.686	-103.008	56.280
429.78	29.729	49.727	40.812	3.831	-130.589	-100.951	51.334
429.78	29.729	49.727	40.812	3.831	-132.149	-100.951	51.334
500	30.200	54.267	42.391	5.938	-131.906	-95.871	41.905
600	30.630	59.813	44.845	8.981	-131.538	-88.698	32.308
660	30.828	62.742	46.340	10.825	-131.308	-84.425	27.956
660	32.060	63.151	46.340	11.095	-131.038	-84.425	27.956
700	32.600	65.054	47.357	12.388	-130.823	-81.607	25.479
800	33.952	69.495	49.850	15.716	-130.198	-74.616	20.384
900	35.304	73.572	52.262	19.179	-129.447	-67.713	16.443
1000	36.657	77.362	54.585	22.777	-128.569	-60.899	13.309
1100	38.009	80.919	56.819	26.510	-127.569	-54.179	10.764
1100	38.300	81.801	56.819	27.480	-126.599	-54.179	10.764
1200	38.300	85.133	59.041	31.310	-125.512	-47.644	8.677
1300	38.300	88.199	61.168	35.140	-124.435	-41.201	6.926

Phase changes: 429.78 K, melting point of In; ΔH° = 0.780 kcal/mol.
660 K, α - β transition point of In₂S₃; ΔH° = 0.270 kcal/mol.
1100 K, β - γ transition point of In₂S₃; ΔH° = 0.970 kcal/mol.

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

298.15-660 K: Cp° = 30.434 + 1.416x10⁻³T - 2.356x10⁻⁵T²
H° - H₂₉₈° = 30.434x10⁻³T + 0.708x10⁻⁶T² + 2.356x10⁻²T⁻¹ - 9.927
660-1100 K: Cp° = 23.188 + 13.478x10⁻³T - 0.100x10⁻⁵T²
H° - H₂₉₈° = 23.188x10⁻³T + 6.739x10⁻⁶T² + 0.100x10⁻²T⁻¹ - 7.160
1100-1300 K: Cp° = 38.300
H° - H₂₉₈° = 38.300x10⁻³T - 14.650

Reaction equations (kcal/mol):

298.15-429.78 K: ΔHr° = -135.020 + 12.679x10⁻³T - 9.296x10⁻⁶T² + 298.550T⁻¹
ΔGr° = -135.020 - 12.679x10⁻³TlnT + 9.296x10⁻⁶T² + 149.275T⁻¹ + 151.357x10⁻³T
429.78-660 K: ΔHr° = -134.301 + 3.985x10⁻³T + 0.248x10⁻⁶T² + 167.150T⁻¹
ΔGr° = -134.301 - 3.985x10⁻³TlnT - 0.248x10⁻⁶T² + 83.575T⁻¹ + 101.427x10⁻³T
660-1100 K: ΔHr° = -131.534 - 3.261x10⁻³T + 6.279x10⁻⁶T² - 58.450T⁻¹
ΔGr° = -131.534 + 3.261x10⁻³TlnT - 6.279x10⁻⁶T² - 29.225T⁻¹ + 54.431x10⁻³T
1100-1300 K: ΔHr° = -139.024 + 11.851x10⁻³T - 0.460x10⁻⁶T² - 68.450T⁻¹
ΔGr° = -139.024 - 11.851x10⁻³TlnT + 0.460x10⁻⁶T² - 34.225T⁻¹ + 159.662x10⁻³T

Sources: Enthalpy of formation at 298 K from Mills (80). Low-temperature heat capacities and entropy at 298 K from King (68). High-temperature data based on Pankratz (90).

IrS₂(c)
Iridium Disulfide
[Formation: Ir(c) + 2S(c,l) = IrS₂(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15*	15.740	17.000	17.000	0	-31.400	-29.372	21.530
300	15.750	17.100	17.000	.030	-31.401	-29.359	21.387
368.3	16.255	20.378	17.334	1.121	-31.490	-28.887	17.141
368.3	16.255	20.378	17.334	1.121	-31.682	-28.887	17.141
388.36	16.404	21.244	17.514	1.449	-31.714	-28.732	16.169
388.36	16.404	21.244	17.514	1.449	-32.540	-28.732	16.169
400	16.490	21.730	17.630	1.640	-32.596	-28.618	15.636
432.02	16.724	23.009	17.982	2.172	-32.786	-28.293	14.313
500	17.220	25.490	18.830	3.330	-33.396	-27.528	12.032
600	17.950	28.690	20.207	5.090	-33.980	-26.292	9.577
700	18.690	31.510	21.624	6.920	-34.393	-24.977	7.798
717.824	18.820	31.981	21.876	7.254	-34.449	-24.735	7.531

*Data except enthalpy of formation at 298 K estimated.

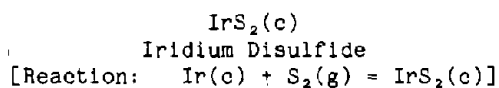
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1400 K: Cp° = 13.550 + 7.340x10⁻³T
H°- H₂₉₈° = 13.550x10⁻³T + 3.670x10⁻⁶T² - 4.366

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -28.496 - 8.246x10⁻³T + 6.365x10⁻⁶T² - 301.600T⁻¹
ΔGf° = -28.496 + 8.246x10⁻³TlnT - 6.365x10⁻⁶T² - 150.800T⁻¹ - 46.326x10⁻³T
368.3-388.36 K: ΔHf° = -30.726 - 3.720x10⁻³T + 2.873x10⁻⁶T² + 9.600T⁻¹
ΔGf° = -30.726 + 3.720x10⁻³TlnT - 2.873x10⁻⁶T² + 4.800T⁻¹ - 15.960x10⁻³T
388.36-432.02 K: ΔHf° = -63.043 + 85.760x10⁻³T - 83.691x10⁻⁶T² + 3814.000T⁻¹
ΔGf° = -63.043 - 85.760x10⁻³TlnT + 83.691x10⁻⁶T² + 1907.000T⁻¹ + 554.496x10⁻³T
432.02-717.824 K: ΔHf° = -82.000 + 77.948x10⁻³T - 44.067x10⁻⁶T² + 10267.000T⁻¹
ΔGf° = -82.000 - 77.948x10⁻³TlnT + 44.067x10⁻⁶T² + 5133.500T⁻¹ + 550.801x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHr°	ΔGr°	
298.15*	15.740	17.000	17.000	0	-62.110	-48.399	35.477
300	15.750	17.100	17.000	.030	-62.105	-48.313	35.196
400	16.490	21.730	17.630	1.640	-61.898	-43.749	23.903
500	17.220	25.490	18.830	3.330	-61.651	-39.234	17.149
600	17.950	28.690	20.207	5.090	-61.369	-34.774	12.666
700	18.690	31.510	21.624	6.920	-61.043	-30.367	9.481
800	19.420	34.060	23.035	8.820	-60.671	-26.020	7.108
900	20.160	36.390	24.390	10.800	-60.242	-21.713	5.273
1000	20.890	38.550	25.700	12.850	-59.764	-17.457	3.815
1100	21.620	40.570	26.952	14.980	-59.229	-13.241	2.631
1200	22.360	42.490	28.173	17.180	-58.646	-9.094	1.656
1300	23.090	44.310	29.348	19.450	-58.015	-4.996	.840
1400	23.830	46.040	30.469	21.800	-57.326	-.926	.144

*Data except enthalpy of formation at 298 K estimated.

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

298.15-1400 K: $\text{Cp}^\circ = 13.550 + 7.340 \times 10^{-3} \text{T}$
 $\text{H}^\circ - \text{H}_{298}^\circ = 13.550 \times 10^{-3} \text{T} + 3.670 \times 10^{-6} \text{T}^2 - 4.366$

Reaction equations (kcal/mol):

298.15-1400 K: $\Delta\text{Hr}^\circ = -62.073 - 0.241 \times 10^{-3} \text{T} + 2.611 \times 10^{-6} \text{T}^2 - 58.700 \text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -62.073 + 0.241 \times 10^{-3} \text{T} \ln \text{T} - 2.611 \times 10^{-6} \text{T}^2 - 29.350 \text{T}^{-1} + 45.600 \times 10^{-3} \text{T}$

Source: Data from Chang (16) who estimated all except enthalpy of formation at 298 K.

$\text{Ir}_2\text{S}_3(\text{c})$
 Diiridium Trisulfide
 [Formation: $2\text{Ir}(\text{c}) + 3\text{S}(\text{c},1) = \text{Ir}_2\text{S}_3(\text{c})$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHf°	ΔGf°	
298.15*	27.430	29.300	29.300	0	-49.300	-46.126	33.811
300	27.450	29.470	29.303	.050	-49.302	-46.107	33.588
368.3	28.167	35.171	29.871	1.952	-49.376	-45.371	26.923
368.3	28.167	35.171	29.871	1.952	-49.664	-45.371	26.923
388.36	28.378	36.670	30.184	2.519	-49.698	-45.134	25.399
388.36	28.378	36.670	30.184	2.519	-50.937	-45.134	25.399
400	28.500	37.510	30.385	2.850	-51.012	-44.960	24.564
432.02	28.836	39.718	30.996	3.768	-51.275	-44.467	22.495
500	29.550	43.980	32.480	5.750	-52.155	-43.317	18.934
600	30.600	49.460	34.860	8.760	-52.976	-41.466	15.104
700	31.650	54.260	37.303	11.870	-53.552	-39.504	12.334
717.824	31.837	55.058	37.734	12.436	-53.629	-39.144	11.918

*Data except enthalpy of formation at 298 K estimated.

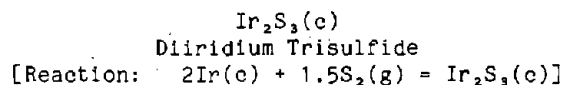
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta\text{H}^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta\text{H}^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta\text{H}^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-1200 K: $\text{Cp}^\circ = 24.300 + 10.500 \times 10^{-3} \text{T}$
 $\text{H}^\circ - \text{H}_{298}^\circ = 24.300 \times 10^{-3} \text{T} + 5.250 \times 10^{-6} \text{T}^2 - 7.712$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta\text{Hf}^\circ = -45.277 - 11.118 \times 10^{-3} \text{T} + 8.923 \times 10^{-6} \text{T}^2 - 447.600 \text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -45.277 + 11.118 \times 10^{-3} \text{T} \ln \text{T} - 8.923 \times 10^{-6} \text{T}^2 - 223.800 \text{T}^{-1} - 61.016 \times 10^{-3} \text{T}$
 368.3-388.36 K: $\Delta\text{Hf}^\circ = -48.622 - 4.329 \times 10^{-3} \text{T} + 3.685 \times 10^{-6} \text{T}^2 + 19.200 \text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -48.622 + 4.329 \times 10^{-3} \text{T} \ln \text{T} - 3.685 \times 10^{-6} \text{T}^2 + 9.600 \text{T}^{-1} - 15.467 \times 10^{-3} \text{T}$
 388.36-432.02 K: $\Delta\text{Hf}^\circ = -97.097 + 129.891 \times 10^{-3} \text{T} - 126.161 \times 10^{-6} \text{T}^2 + 5725.800 \text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -97.097 - 129.891 \times 10^{-3} \text{T} \ln \text{T} + 126.161 \times 10^{-6} \text{T}^2 + 2862.900 \text{T}^{-1} + 840.218 \times 10^{-3} \text{T}$
 432.02-717.82 K: $\Delta\text{Hf}^\circ = -125.533 + 118.173 \times 10^{-3} \text{T} - 66.725 \times 10^{-6} \text{T}^2 + 15405.300 \text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -125.533 - 118.173 \times 10^{-3} \text{T} \ln \text{T} + 66.725 \times 10^{-6} \text{T}^2 + 7702.650 \text{T}^{-1} + 834.676 \times 10^{-3} \text{T}$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHr°	ΔGr°	
298.15*	27.430	29.300	29.300	0	-95.365	-74.667	54.732
300	27.450	29.470	29.303	.050	-95.358	-74.538	54.301
400	28.500	37.510	30.385	2.850	-94.965	-67.656	36.965
500	29.550	43.980	32.480	5.750	-94.537	-60.877	26.609
600	30.600	49.460	34.860	8.760	-94.060	-54.188	19.738
700	31.650	54.260	37.303	11.870	-93.527	-47.590	14.858
800	32.700	58.550	39.688	15.090	-92.928	-41.060	11.217
900	33.750	62.470	42.014	18.410	-92.270	-34.625	8.408
1000	34.800	66.080	44.240	21.840	-91.540	-28.254	6.175
1100	35.850	69.440	46.376	25.370	-90.753	-21.960	4.363
1200	36.900	72.610	48.435	29.010	-89.896	-15.749	2.868

*Data except enthalpy of formation at 298 K estimated.

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

298.15-1200 K: $\text{Cp}^\circ = 24.300 + 10.500 \times 10^{-3} \text{T}$
 $\text{H}^\circ - \text{H}_{298}^\circ = 24.300 \times 10^{-3} \text{T} + 5.250 \times 10^{-6} \text{T}^2 - 7.712$

Reaction equations (kcal/mol):

298.15-1200 K: $\Delta\text{Hr}^\circ = -95.644 + 0.889 \times 10^{-3} \text{T} + 3.292 \times 10^{-6} \text{T}^2 - 83.250 \text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -95.644 - 0.889 \times 10^{-3} \text{T} \ln \text{T} - 3.292 \times 10^{-6} \text{T}^2 - 41.625 \text{T}^{-1} + 76.873 \times 10^{-3} \text{T}$

Source: Data from Chang (15) who estimated all except enthalpy of formation at 298 K.

KS(g)
Potassium Monosulfide (ideal gas)
[Formation: $K(c,l) + S(c,l) = KS(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15*	8.652	59.546	59.546	0	26.600	15.739	-11.537
300	8.655	59.599	59.546	.016	26.593	15.672	-11.417
336.35	8.701	60.592	59.606	.331	26.436	14.357	-9.329
336.35	8.701	60.592	59.606	.331	25.878	14.357	-9.329
368.3	8.742	61.385	59.725	.611	25.730	13.270	-7.874
368.3	8.742	61.385	59.725	.611	25.634	13.270	-7.874
388.36	8.767	61.849	59.823	.787	25.539	12.600	-7.090
388.36	8.767	61.849	59.823	.787	25.126	12.600	-7.090
400	8.782	62.108	59.886	.889	25.052	12.225	-6.679
432.02	8.802	62.785	60.076	1.171	24.830	11.206	-5.669
500	8.845	64.076	60.536	1.770	24.253	9.109	-3.981
600	8.883	65.692	61.264	2.657	23.557	6.148	-2.239
700	8.907	67.063	61.997	3.546	22.930	3.296	-1.029
717.824	8.910	67.287	62.126	3.705	22.825	2.798	-.852

*Data except enthalpy of formation at 298 K estimated.

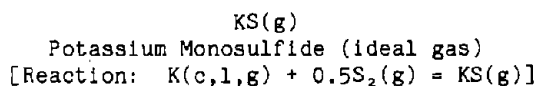
Phase changes: 336.35 K, melting point of K; $\Delta H^\circ = 0.558$ kcal/mol.
 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: $C_p^\circ = 8.921 + 0.048 \times 10^{-3}T - 0.252 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 8.921 \times 10^{-3}T + 0.024 \times 10^{-6}T^2 + 0.252 \times 10^{-2}T^{-1} - 2.746$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta H_f^\circ = 27.867 - 0.299 \times 10^{-3}T - 8.327 \times 10^{-6}T^2 - 130.400T^{-1}$
 $\Delta G_f^\circ = 27.867 + 0.299 \times 10^{-3}T \ln T + 8.327 \times 10^{-6}T^2 - 65.200T^{-1} - 44.129 \times 10^{-3}T$
 336.35-368.3 K: $\Delta H_f^\circ = 27.870 - 6.098 \times 10^{-3}T + 1.625 \times 10^{-6}T^2 - 41.800T^{-1}$
 $\Delta G_f^\circ = 27.870 + 6.098 \times 10^{-3}T \ln T - 1.625 \times 10^{-6}T^2 - 20.900T^{-1} - 74.923 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = 26.755 - 3.835 \times 10^{-3}T - 0.121 \times 10^{-6}T^2 + 113.800T^{-1}$
 $\Delta G_f^\circ = 26.755 + 3.835 \times 10^{-3}T \ln T + 0.121 \times 10^{-6}T^2 + 56.900T^{-1} - 59.740 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = 10.596 + 40.905 \times 10^{-3}T - 43.403 \times 10^{-6}T^2 + 2016.000T^{-1}$
 $\Delta G_f^\circ = 10.596 - 40.905 \times 10^{-3}T \ln T + 43.403 \times 10^{-6}T^2 + 1008.000T^{-1} + 225.489 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = 1.118 + 36.999 \times 10^{-3}T - 23.591 \times 10^{-6}T^2 + 5242.500T^{-1}$
 $\Delta G_f^\circ = 1.118 - 36.999 \times 10^{-3}T \ln T + 23.591 \times 10^{-6}T^2 + 2621.250T^{-1} + 223.641 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	8.652	59.546	59.546	0	11.245	6.225	-4.563
300	8.655	59.599	59.546	.016	11.241	6.195	-4.513
336.35	8.701	60.592	59.606	.331	11.143	5.589	-3.631
336.35	8.701	60.592	59.606	.331	10.585	5.589	-3.631
400	8.782	62.108	59.886	.889	10.401	4.660	-2.546
500	8.845	64.076	60.536	1.770	10.126	3.255	-1.423
600	8.883	65.692	61.264	2.657	9.863	1.907	-.695
700	8.907	67.063	61.997	3.546	9.605	.601	-.188
800	8.924	68.254	62.706	4.438	9.349	-.668	.182
900	8.937	69.305	63.382	5.331	9.090	-1.904	.462
1000	8.947	70.248	64.023	6.225	8.820	-3.113	.680
1043.7	8.950	70.631	64.292	6.616	8.697	-3.630	.760
1043.7	8.950	70.631	64.292	6.616	-10.341	-3.630	.760
1100	8.955	71.101	64.628	7.120	-10.369	-3.268	.649
1200	8.962	71.880	65.200	8.016	-10.422	-2.618	.477
1300	8.969	72.598	65.742	8.913	-10.475	-1.967	.331
1400	8.975	73.263	66.256	9.810	-10.534	-1.309	.204
1500	8.980	73.882	66.743	10.708	-10.594	-.647	.094
1600	8.985	74.462	67.208	11.606	-10.660	.017	-.002
1700	8.990	75.007	67.651	12.505	-10.728	.685	-.088
1800	8.994	75.521	68.074	13.404	-10.799	1.359	-.165
1900	8.998	76.007	68.479	14.304	-10.874	2.037	-.234
2000	9.002	76.469	68.867	15.204	-10.953	2.718	-.298

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.

1043.7 K, calculated boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.

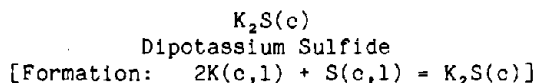
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 8.921 + 0.048 \times 10^{-3}T - 0.252 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 8.921 \times 10^{-3}T + 0.024 \times 10^{-6}T^2 + 0.252 \times 10^{-2}T^{-1} - 2.746$

Reaction equations (kcal/mol):

298.15-336.35 K: $\Delta H_r^\circ = 11.078 + 3.703 \times 10^{-3}T - 10.204 \times 10^{-6}T^2 - 8.950T^{-1}$
 $\Delta G_r^\circ = 11.078 - 3.703 \times 10^{-3}T \ln T + 10.204 \times 10^{-6}T^2 - 4.475T^{-1} + 1.834 \times 10^{-3}T$
336.35-1043.7 K: $\Delta H_r^\circ = 11.081 - 2.096 \times 10^{-3}T - 0.252 \times 10^{-6}T^2 + 79.650T^{-1}$
 $\Delta G_r^\circ = 11.081 + 2.096 \times 10^{-3}T \ln T + 0.252 \times 10^{-6}T^2 + 39.825T^{-1} - 28.960 \times 10^{-3}T$
1043.7-2000 K: $\Delta H_r^\circ = -10.522 + 0.242 \times 10^{-3}T - 0.258 \times 10^{-6}T^2 + 216.650T^{-1}$
 $\Delta G_r^\circ = -10.522 - 0.242 \times 10^{-3}T \ln T + 0.258 \times 10^{-6}T^2 + 108.325T^{-1} + 7.920 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Farber (34). Other data are those estimated by Piper (100).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	17.850	27.500	27.500	0	-97.080	-93.778	68.740
300	17.860	27.610	27.500	.033	-97.083	-93.757	68.301
336.35	18.085	29.666	27.625	.686	-97.173	-93.350	60.655
336.35	18.085	29.666	27.625	.686	-98.289	-93.350	60.655
368.3	18.283	31.315	27.874	1.267	-98.381	-92.877	55.113
368.3	18.283	31.315	27.874	1.267	-98.477	-92.877	55.113
388.36	18.408	32.288	28.078	1.635	-98.532	-92.570	52.093
388.36	18.408	32.288	28.078	1.635	-98.945	-92.570	52.093
400	18.480	32.833	28.208	1.850	-98.994	-92.378	50.472
432.02	18.679	34.264	28.604	2.445	-99.142	-91.843	46.461
500	19.100	37.024	29.566	3.729	-99.538	-90.662	39.628
600	19.720	40.561	31.111	5.670	-99.906	-88.847	32.362
700	20.350	43.648	32.687	7.673	-100.135	-86.985	27.158
717.824	20.460	44.161	32.965	8.037	-100.162	-86.649	26.381

*Entropy at 298 K estimated.

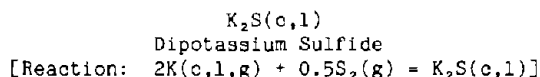
Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1050 K: $C_p^\circ = -3.365 + 33.940 \times 10^{-3}T + 9.863 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = -3.365 \times 10^{-3}T + 16.970 \times 10^{-6}T^2 - 9.863 \times 10^{-2}T^{-1} + 2.803$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta H_f^\circ = -89.057 - 13.631 \times 10^{-3}T - 1.449 \times 10^{-6}T^2 - 1141.900T^{-1}$
 $\Delta G_f^\circ = -89.057 + 13.631 \times 10^{-3}T \ln T + 1.449 \times 10^{-6}T^2 - 570.950T^{-1} - 87.507 \times 10^{-3}T$
 336.35-368.3 K: $\Delta H_f^\circ = -89.051 - 25.229 \times 10^{-3}T + 18.455 \times 10^{-6}T^2 - 964.700T^{-1}$
 $\Delta G_f^\circ = -89.051 + 25.229 \times 10^{-3}T \ln T - 18.455 \times 10^{-6}T^2 - 482.350T^{-1} - 149.093 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -90.166 - 22.966 \times 10^{-3}T + 16.709 \times 10^{-6}T^2 - 809.100T^{-1}$
 $\Delta G_f^\circ = -90.166 + 22.966 \times 10^{-3}T \ln T - 16.709 \times 10^{-6}T^2 - 404.550T^{-1} - 133.910 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -106.324 + 21.774 \times 10^{-3}T - 26.573 \times 10^{-6}T^2 + 1093.100T^{-1}$
 $\Delta G_f^\circ = -106.324 - 21.774 \times 10^{-3}T \ln T + 26.573 \times 10^{-6}T^2 + 546.550T^{-1} + 151.318 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -115.803 + 17.868 \times 10^{-3}T - 6.761 \times 10^{-6}T^2 + 4319.600T^{-1}$
 $\Delta G_f^\circ = -115.803 - 17.868 \times 10^{-3}T \ln T + 6.761 \times 10^{-6}T^2 + 2159.800T^{-1} + 149.471 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	17.850	27.500	27.500	0	-112.435	-103.292	75.714
300	17.860	27.610	27.500	.033	-112.435	-103.234	75.205
336.35	18.085	29.666	27.625	.686	-112.466	-102.118	66.352
336.35	18.085	29.666	27.625	.686	-113.582	-102.118	66.352
400	18.480	32.833	28.208	1.850	-113.645	-99.944	54.606
500	19.100	37.024	29.566	3.729	-113.666	-96.515	42.186
600	19.720	40.561	31.111	5.670	-113.601	-93.088	33.907
700	20.350	43.648	32.687	7.673	-113.460	-89.680	27.999
800	20.970	46.406	34.232	9.739	-113.254	-86.297	23.575
900	24.750	49.020	35.728	11.963	-112.894	-82.944	20.141
1000	37.300	52.169	37.207	14.962	-111.780	-79.667	17.411
1043.7	45.428	53.923	37.874	16.750	-110.825	-78.286	16.393
1043.7	45.428	53.923	37.874	16.750	-148.901	-78.286	16.393
1050	46.600	54.200	37.971	17.040	-148.702	-77.860	16.206
1100	34.020	56.061	38.749	19.043	-147.421	-74.515	14.805
1200	34.020	59.021	40.317	22.445	-145.464	-67.972	12.379
1221	34.020	59.612	40.644	23.160	-145.052	-66.620	11.924
1221	24.130	62.773	40.644	27.020	-141.192	-66.620	11.924
1300	24.130	64.285	42.034	28.926	-140.429	-61.818	10.392
1400	24.130	66.073	43.688	31.339	-139.469	-55.805	8.711
1500	24.130	67.738	45.237	33.752	-138.512	-49.862	7.265
1600	24.130	69.295	46.692	36.165	-137.560	-43.984	6.008
1700	24.130	70.758	48.065	38.578	-136.611	-38.166	4.907
1800	24.130	72.138	49.365	40.991	-135.667	-32.404	3.934
1900	24.130	73.442	50.598	43.404	-134.728	-26.691	3.070
2000	24.130	74.680	51.771	45.817	-133.796	-21.029	2.298

*Entropy at 298 K estimated.

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
1043.7 K, calculated boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.
1050 K, second order transition point of K₂; ΔH° = 0 kcal/mol.
1221 K, melting point of K₂; ΔH° = 3.860 kcal/mol.

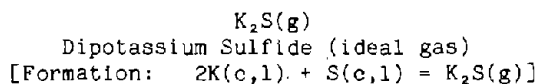
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1050 K: Cp° = -3.365 + 33.940x10⁻³T + 9.863x10⁻⁵T²
H° - H₂₉₈° = -3.365x10⁻³T + 16.970x10⁻⁶T² - 9.863x10⁻²T⁻¹ + 2.803
1050-1221 K: Cp° = 62.160 - 23.224x10⁻³T
H° - H₂₉₈° = 62.160x10⁻³T - 11.612x10⁻⁶T² - 35.426
1221-2000 K: Cp° = 24.130
H° - H₂₉₈° = 24.130x10⁻³T - 2.443

Reaction equations (kcal/mol):

298.15-336.35 K: ΔHr° = -105.846 - 9.628x10⁻³T - 3.326x10⁻⁶T² - 1020.450T⁻¹
ΔGr° = -105.846 + 9.628x10⁻³TlnT + 3.326x10⁻⁶T² - 510.225T⁻¹ - 41.544x10⁻³T
336.35-1043.7 K: ΔHr° = -105.840 - 21.227x10⁻³T + 16.578x10⁻⁶T² - 843.250T⁻¹
ΔGr° = -105.840 + 21.227x10⁻³TlnT - 16.578x10⁻⁶T² - 421.625T⁻¹ - 103.130x10⁻³T
1043.7-1050 K: ΔHr° = -149.045 - 16.551x10⁻³T + 16.566x10⁻⁶T² - 569.250T⁻¹
ΔGr° = -149.045 + 16.551x10⁻³TlnT - 16.566x10⁻⁶T² - 284.625T⁻¹ - 29.371x10⁻³T
1050-1221 K: ΔHr° = -187.274 + 48.974x10⁻³T - 12.016x10⁻⁶T² + 417.050T⁻¹
ΔGr° = -187.274 - 48.974x10⁻³TlnT + 12.016x10⁻⁶T² + 208.525T⁻¹ + 432.407x10⁻³T
1221-2000 K: ΔHr° = -154.291 + 10.944x10⁻³T - 0.404x10⁻⁶T² + 417.050T⁻¹
ΔGr° = -154.291 - 10.944x10⁻³TlnT + 0.404x10⁻⁶T² + 208.525T⁻¹ + 149.276x10⁻³T

Sources: Enthalpy of formation at 298 K from Johnson (57). Other data from Chase (17) who estimated entropy at 298 K.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15*	13.236	72.100	72.100	0	-3.700	-13.695	10.039
300	13.242	72.182	72.102	.024	-3.712	-13.757	10.022
336.35	13.342	73.702	72.194	.507	-3.972	-14.960	9.721
336.35	13.342	73.702	72.194	.507	-5.088	-14.960	9.721
368.3	13.430	74.922	72.378	.937	-5.331	-15.887	9.427
368.3	13.430	74.922	72.378	.937	-5.427	-15.887	9.427
388.36	13.485	75.635	72.528	1.207	-5.581	-16.452	9.258
388.36	13.485	75.635	72.528	1.207	-5.994	-16.452	9.258
400	13.517	76.034	72.624	1.364	-6.100	-16.764	9.160
432.02	13.561	77.077	72.916	1.798	-6.410	-17.607	8.907
500	13.653	79.066	73.620	2.723	-7.164	-19.309	8.440
600	13.730	81.563	74.741	4.093	-8.103	-21.646	7.884
700	13.777	83.683	75.872	5.468	-8.960	-23.834	7.441
717.824	13.783	84.029	76.070	5.714	-9.105	-24.211	7.371

*Data except enthalpy of formation at 298 K estimated.

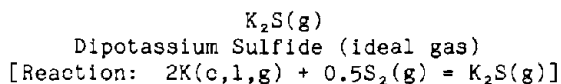
Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 13.859 + 0.036x10⁻³T - 0.563x10⁻⁵T⁻²
 H°- H₂₉₈° = 13.859x10⁻³T + 0.018x10⁻⁶T² + 0.563x10⁻²T⁻¹ - 4.322

Formation equations (kcal/mol):

298.15-336.35 K: ΔHf° = -2.802 + 3.593x10⁻³T - 18.401x10⁻⁶T² - 99.300T⁻¹
 ΔGf° = -2.802 - 3.593x10⁻³TlnT + 18.401x10⁻⁶T² - 49.650T⁻¹ - 20.992x10⁻³T
 336.35-368.3 K: ΔHf° = -2.796 - 8.005x10⁻³T + 1.503x10⁻⁶T² + 77.900T⁻¹
 ΔGf° = -2.796 + 8.005x10⁻³TlnT - 1.503x10⁻⁶T² + 38.950T⁻¹ - 82.578x10⁻³T
 368.3-388.36 K: ΔHf° = -3.911 - 5.742x10⁻³T - 0.243x10⁻⁶T² + 233.500T⁻¹
 ΔGf° = -3.911 + 5.742x10⁻³TlnT + 0.243x10⁻⁶T² + 116.750T⁻¹ - 67.395x10⁻³T
 388.36-432.02 K: ΔHf° = -20.070 + 38.998x10⁻³T - 43.525x10⁻⁶T² + 2135.700T⁻¹
 ΔGf° = -20.070 - 38.998x10⁻³TlnT + 43.525x10⁻⁶T² + 1067.850T⁻¹ + 217.833x10⁻³T
 432.02-717.824 K: ΔHf° = -29.548 + 35.092x10⁻³T - 23.713x10⁻⁶T² + 5362.200T⁻¹
 ΔGf° = -29.548 - 35.092x10⁻³TlnT + 23.713x10⁻⁶T² + 2681.100T⁻¹ + 215.986x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15*	13.236	72.100	72.100	0	-19.055	-23.209	17.013
300	13.242	72.182	72.102	.024	-19.064	-23.235	16.926
336.35	13.342	73.702	72.194	.507	-19.265	-23.729	15.418
336.35	13.342	73.702	72.194	.507	-20.381	-23.729	15.418
400	13.517	76.034	72.624	1.364	-20.751	-24.330	13.293
500	13.653	79.066	73.620	2.723	-21.291	-25.162	10.998
600	13.730	81.563	74.741	4.093	-21.798	-25.887	9.429
700	13.777	83.683	75.872	5.468	-22.285	-26.529	8.283
800	13.808	85.525	76.965	6.848	-22.764	-27.103	7.404
900	13.829	87.153	78.009	8.230	-23.247	-27.617	6.706
1000	13.844	88.611	78.998	9.613	-23.749	-28.077	6.136
1043.7	13.849	89.203	79.413	10.218	-23.977	-28.260	5.918
1043.7	13.849	89.203	79.413	10.218	-62.053	-28.260	5.918
1100	13.856	89.931	79.933	10.998	-62.085	-26.437	5.252
1200	13.864	91.137	80.817	12.384	-62.145	-23.192	4.224
1300	13.871	92.247	81.654	13.771	-62.204	-19.944	3.353
1400	13.876	93.275	82.447	15.159	-62.269	-16.687	2.605
1500	13.881	94.232	83.201	16.546	-62.338	-13.429	1.957
1600	13.884	95.128	83.919	17.935	-62.410	-10.167	1.389
1700	13.887	95.970	84.604	19.323	-62.485	-6.901	.887
1800	13.890	96.764	85.257	20.712	-62.567	-3.630	.441
1900	13.892	97.515	85.883	22.101	-62.651	-.353	.041
2000	13.894	98.228	86.483	23.490	-62.743	2.928	-.320

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.

1043.7 K, calculated boiling point of K to ideal monatomic gas; ΔH° = 19.038 kcal/mol.

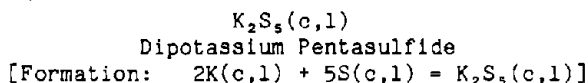
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 13.859 + 0.036 \times 10^{-3}T - 0.563 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 13.859 \times 10^{-3}T + 0.018 \times 10^{-6}T^2 + 0.563 \times 10^{-2}T^{-1} - 4.322$

Reaction equations (kcal/mol):

298.15-336.35 K: $\Delta H_r^\circ = -19.591 + 7.595 \times 10^{-3}T - 20.278 \times 10^{-6}T^2 + 22.150T^{-1}$
 $\Delta G_r^\circ = -19.591 - 7.595 \times 10^{-3}T \ln T + 20.278 \times 10^{-6}T^2 + 11.075T^{-1} + 24.971 \times 10^{-3}T$
336.35-1043.7 K: $\Delta H_r^\circ = -19.585 - 4.003 \times 10^{-3}T - 0.374 \times 10^{-6}T^2 + 199.350T^{-1}$
 $\Delta G_r^\circ = -19.585 + 4.003 \times 10^{-3}T \ln T + 0.374 \times 10^{-6}T^2 + 99.675T^{-1} - 36.615 \times 10^{-3}T$
1043.7-2000 K: $\Delta H_r^\circ = -62.791 + 0.673 \times 10^{-3}T - 0.386 \times 10^{-6}T^2 + 473.350T^{-1}$
 $\Delta G_r^\circ = -62.791 - 0.673 \times 10^{-3}T \ln T + 0.386 \times 10^{-6}T^2 + 236.675T^{-1} + 37.144 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Farber (34). Other data are those estimated by Piper (100).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	43.410	62.000	62.000	0	-112.100	-109.948	80.593
300	43.550	62.270	62.003	.080	-112.096	-109.934	80.086
336.35	46.138	67.395	62.301	1.714	-112.012	-109.675	71.262
336.35	46.138	67.395	62.301	1.714	-113.128	-109.675	71.262
350	47.110	69.250	62.536	2.350	-113.088	-109.535	68.396
368.3	48.351	71.683	62.930	3.223	-113.020	-109.352	64.889
368.3	48.351	71.683	62.930	3.223	-113.500	-109.352	64.889
388.36	49.711	74.280	63.448	4.207	-113.417	-109.124	61.409
388.36	49.711	74.280	63.448	4.207	-115.482	-109.124	61.409
400	50.500	75.760	63.785	4.790	-115.514	-108.934	59.518
432.02	52.568	79.733	64.816	6.444	-115.655	-108.403	54.838
450	53.730	81.900	65.456	7.400	-116.078	-108.093	52.496
478	55.450	85.200	66.537	8.920	-116.165	-107.598	49.195
478	69.370	98.690	66.537	15.370	-109.715	-107.598	49.195
500	69.370	101.810	68.010	16.900	-109.575	-107.497	46.987
550	69.370	108.420	71.384	20.370	-109.013	-107.310	42.640
600	69.370	114.460	74.727	23.840	-108.372	-107.184	39.041
650	69.370	120.010	78.010	27.300	-107.655	-107.120	36.017

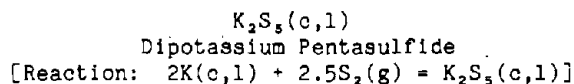
Phase changes: 336.35 K, melting point of K; $\Delta H^\circ = 0.558$ kcal/mol.
 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 478 K, melting point of K_2S_5 ; $\Delta H^\circ = 6.450$ kcal/mol.

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

298.15-478 K: $C_p^\circ = 30.227 + 55.154 \times 10^{-3}T - 2.899 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 30.227 \times 10^{-3}T + 27.577 \times 10^{-6}T^2 + 2.899 \times 10^{-2}T^3 - 12.436$
 478-650 K: $C_p^\circ = 69.370$
 $H^\circ - H_{298}^\circ = 69.370 \times 10^{-3}T - 17.789$

Formation equations (kcal/mol):

298.15-336.35 K: $\Delta H_f^\circ = -108.091 - 12.735 \times 10^{-3}T + 16.026 \times 10^{-6}T^2 - 488.100T^{-1}$
 $\Delta G_f^\circ = -108.091 + 12.735 \times 10^{-3}T \ln T - 16.026 \times 10^{-6}T^2 - 244.050T^{-1} - 71.264 \times 10^{-3}T$
 336.35-368.3 K: $\Delta H_f^\circ = -108.084 - 24.333 \times 10^{-3}T + 35.930 \times 10^{-6}T^2 - 310.900T^{-1}$
 $\Delta G_f^\circ = -108.084 + 24.333 \times 10^{-3}T \ln T - 35.930 \times 10^{-6}T^2 - 155.450T^{-1} - 132.850 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -113.660 - 13.018 \times 10^{-3}T + 27.200 \times 10^{-6}T^2 + 467.100T^{-1}$
 $\Delta G_f^\circ = -113.660 + 13.018 \times 10^{-3}T \ln T - 27.200 \times 10^{-6}T^2 + 233.550T^{-1} - 56.936 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -194.451 + 210.682 \times 10^{-3}T - 189.210 \times 10^{-6}T^2 + 9978.100T^{-1}$
 $\Delta G_f^\circ = -194.451 - 210.682 \times 10^{-3}T \ln T + 189.210 \times 10^{-6}T^2 + 4989.050T^{-1} + 1369.206 \times 10^{-3}T$
 432.02-478 K: $\Delta H_f^\circ = -241.845 + 191.152 \times 10^{-3}T - 90.150 \times 10^{-6}T^2 + 26110.600T^{-1}$
 $\Delta G_f^\circ = -241.845 - 191.152 \times 10^{-3}T \ln T + 90.150 \times 10^{-6}T^2 + 13055.300T^{-1} + 1359.969 \times 10^{-3}T$
 478-650 K: $\Delta H_f^\circ = -247.198 + 230.295 \times 10^{-3}T - 117.727 \times 10^{-6}T^2 + 25820.700T^{-1}$
 $\Delta G_f^\circ = -247.198 - 230.295 \times 10^{-3}T \ln T + 117.727 \times 10^{-6}T^2 + 12910.350T^{-1} + 1600.117 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	43.410	62.000	62.000	0	-188.875	-157.516	115.461
300	43.550	62.270	62.003	.080	-188.856	-157.320	114.606
336.35	46.138	67.395	62.301	1.714	-188.477	-153.517	99.749
336.35	46.138	67.395	62.301	1.714	-189.593	-153.517	99.749
350	47.110	69.250	62.536	2.350	-189.442	-152.059	94.949
400	50.500	75.760	63.785	4.790	-188.769	-146.762	80.186
450	53.730	81.900	65.456	7.400	-187.933	-141.557	68.749
478	55.450	85.200	66.537	8.920	-187.409	-138.698	63.414
478	69.370	98.690	66.537	15.370	-180.959	-138.698	63.414
500	69.370	101.810	68.010	16.900	-180.212	-136.764	59.779
550	69.370	108.420	71.384	20.370	-178.527	-132.498	52.649
600	69.370	114.460	74.727	23.840	-176.845	-128.389	46.765
650	69.370	120.010	78.010	27.300	-175.175	-124.425	41.835

Phase changes: 336.35 K, melting point of K; ΔH° = 0.558 kcal/mol.
 478 K, melting point of K₂S₅; ΔH° = 6.450 kcal/mol.

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

298.15-478 K: Cp° = 30.227 + 55.154x10⁻³T - 2.899x10⁻⁵T²
 H°- H₂₉₈° = 30.227x10⁻³T + 27.577x10⁻⁶T² + 2.899x10⁻²T³ - 12.436
 478-650 K: Cp° = 69.370
 H°- H₂₉₈° = 69.370x10⁻³T - 17.789

Reaction equations (kcal/mol):

298.15-336.35 K: ΔHr° = -192.035 + 7.277x10⁻³T + 6.641x10⁻⁶T² + 119.150T⁻¹
 ΔGr° = -192.035 - 7.277x10⁻³TlnT - 6.641x10⁻⁶T² + 59.575T⁻¹ + 158.551x10⁻³T
 336.35-478 K: ΔHr° = -192.028 - 4.321x10⁻³T + 26.545x10⁻⁶T² + 296.350T⁻¹
 ΔGr° = -192.028 + 4.321x10⁻³TlnT - 26.545x10⁻⁶T² + 148.175T⁻¹ + 96.965x10⁻³T
 478-650 K: ΔHr° = -197.381 + 34.823x10⁻³T - 1.032x10⁻⁶T² + 6.450T⁻¹
 ΔGr° = -197.381 - 34.823x10⁻³TlnT + 1.032x10⁻⁶T² + 3.225T⁻¹ + 337.113x10⁻³T

Sources: Enthalpy of formation at 298 K from Wagman (127). Low-temperature heat capacities and entropy at 298 K from Diot (29). High-temperature data based on Janz (54).

LaS(c)
Lanthanum Monosulfide
[Formation: $\text{La(c)} + \text{S(c,l)} = \text{LaS(c)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	11.460	16.300	16.300	0	-109.000	-107.521	78.814
300*	11.470	16.370	16.300	.021	-109.001	-107.511	78.321
368.3	11.709	18.749	16.536	.815	-109.036	-107.170	63.594
368.3	11.709	18.749	16.536	.815	-109.132	-107.170	63.594
388.36	11.779	19.372	16.666	1.051	-109.146	-107.061	60.248
388.36	11.779	19.372	16.666	1.051	-109.559	-107.061	60.248
400	11.820	19.720	16.750	1.188	-109.586	-106.986	58.454
432.02	11.884	20.633	17.004	1.568	-109.679	-106.775	54.015
500	12.020	22.390	17.628	2.381	-109.987	-106.294	46.460
550	12.095	23.534	18.108	2.984	-110.150	-105.912	42.085
550	12.095	23.534	18.108	2.984	-110.237	-105.912	42.085
600	12.170	24.590	18.605	3.591	-110.380	-105.513	38.433
700	12.310	26.480	19.601	4.815	-110.634	-104.680	32.682
717.824	12.333	26.790	19.776	5.035	-110.675	-104.527	31.824

*Data above 298 K estimated.

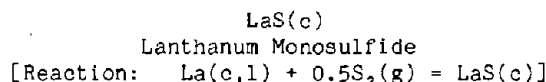
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 550 K, $\alpha - \beta$ transition point of La; $\Delta H^\circ = 0.087$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2500 K: $C_p^\circ = 11.542 + 1.218 \times 10^{-3}T - 0.396 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 11.542 \times 10^{-3}T + 0.609 \times 10^{-6}T^2 + 0.396 \times 10^{-2}T^{-1} - 3.628$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -107.814 - 3.217 \times 10^{-3}T + 2.276 \times 10^{-6}T^2 - 128.000T^{-1}$
 $\Delta G_f^\circ = -107.814 + 3.217 \times 10^{-3}T \ln T - 2.276 \times 10^{-6}T^2 - 64.000T^{-1} - 15.948 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -108.929 - 0.954 \times 10^{-3}T + 0.530 \times 10^{-6}T^2 + 27.600T^{-1}$
 $\Delta G_f^\circ = -108.929 + 0.954 \times 10^{-3}T \ln T - 0.530 \times 10^{-6}T^2 + 13.800T^{-1} - 0.765 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -125.087 + 43.786 \times 10^{-3}T - 42.752 \times 10^{-6}T^2 + 1929.800T^{-1}$
 $\Delta G_f^\circ = -125.087 - 43.786 \times 10^{-3}T \ln T + 42.752 \times 10^{-6}T^2 + 964.900T^{-1} + 284.463 \times 10^{-3}T$
 432.02-550 K: $\Delta H_f^\circ = -134.566 + 39.880 \times 10^{-3}T - 22.940 \times 10^{-6}T^2 + 5156.300T^{-1}$
 $\Delta G_f^\circ = -134.566 - 39.880 \times 10^{-3}T \ln T + 22.940 \times 10^{-6}T^2 + 2578.150T^{-1} + 282.616 \times 10^{-3}T$
 550-717.824 K: $\Delta H_f^\circ = -135.546 + 42.146 \times 10^{-3}T - 24.642 \times 10^{-6}T^2 + 5245.100T^{-1}$
 $\Delta G_f^\circ = -135.546 - 42.146 \times 10^{-3}T \ln T + 24.642 \times 10^{-6}T^2 + 2622.550T^{-1} + 297.613 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	11.460	16.300	16.300	0	-124.355	-117.035	85.788
300*	11.470	16.370	16.300	.021	-124.353	-116.989	85.225
400	11.820	19.720	16.750	1.188	-124.237	-114.552	62.587
500	12.020	22.390	17.628	2.381	-124.115	-112.147	49.019
550	12.095	23.534	18.108	2.984	-124.052	-110.948	44.086
550	12.095	23.534	18.108	2.984	-124.139	-110.948	44.086
600	12.170	24.590	18.605	3.591	-124.074	-109.754	39.977
700	12.310	26.480	19.601	4.815	-123.959	-107.375	33.524
800	12.440	28.130	20.564	6.053	-123.865	-105.014	28.688
900	12.560	29.600	21.486	7.303	-123.795	-102.662	24.929
1000	12.690	30.930	22.364	8.566	-123.748	-100.310	21.922
1100	12.820	32.150	23.204	9.841	-123.728	-97.971	19.465
1134	12.864	32.541	23.478	10.278	-123.726	-97.176	18.728
1134	12.864	32.541	23.478	10.278	-124.472	-97.176	18.728
1193	12.941	33.194	23.942	11.038	-124.536	-95.754	17.541
1193	12.941	33.194	23.942	11.038	-126.017	-95.754	17.541
1200	12.950	33.270	23.996	11.129	-126.016	-95.575	17.406
1300	13.070	34.310	24.748	12.430	-125.989	-93.046	15.642
1400	13.200	35.280	25.463	13.744	-125.953	-90.504	14.128
1500	13.330	36.200	26.153	15.071	-125.909	-87.974	12.818
1600	13.470	37.060	26.803	16.411	-125.854	-85.438	11.670
1700	13.600	37.890	27.440	17.765	-125.790	-82.942	10.663
1800	13.730	38.670	28.042	19.131	-125.716	-80.419	9.764
1900	13.860	39.410	28.615	20.511	-125.631	-77.881	8.958
2000	14.000	40.130	29.178	21.904	-125.537	-75.383	8.237

*Data above 298 K 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.

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

298.15-2500 K: $\text{Cp}^\circ = 11.542 + 1.218 \times 10^{-3}T - 0.396 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 11.542 \times 10^{-3}T + 0.609 \times 10^{-6}T^2 + 0.396 \times 10^{-2}T^{-1} - 3.628$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta \text{Hr}^\circ = -124.603 + 0.785 \times 10^{-3}T + 0.399 \times 10^{-6}T^2 - 6.550T^{-1}$
 $\Delta \text{Gr}^\circ = -124.603 - 0.785 \times 10^{-3}T \ln T - 0.399 \times 10^{-6}T^2 - 3.275T^{-1} + 30.015 \times 10^{-3}T$
550-1134 K: $\Delta \text{Hr}^\circ = -125.583 + 3.051 \times 10^{-3}T - 1.303 \times 10^{-6}T^2 + 82.250T^{-1}$
 $\Delta \text{Gr}^\circ = -125.583 - 3.051 \times 10^{-3}T \ln T + 1.303 \times 10^{-6}T^2 + 41.125T^{-1} + 45.012 \times 10^{-3}T$
1134-1193 K: $\Delta \text{Hr}^\circ = -122.667 - 2.105 \times 10^{-3}T + 0.449 \times 10^{-6}T^2 + 5.450T^{-1}$
 $\Delta \text{Gr}^\circ = -122.667 + 2.105 \times 10^{-3}T \ln T - 0.449 \times 10^{-6}T^2 + 2.725T^{-1} + 8.193 \times 10^{-3}T$
1193-2000 K: $\Delta \text{Hr}^\circ = -125.669 - 0.830 \times 10^{-3}T + 0.449 \times 10^{-6}T^2 + 5.450T^{-1}$
 $\Delta \text{Gr}^\circ = -125.669 + 0.830 \times 10^{-3}T \ln T - 0.449 \times 10^{-6}T^2 + 2.725T^{-1} + 19.742 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (104). Low-temperature heat capacities and entropy at 298 K from Vasilev (123). Data above 298 K estimated.

LaS(g)
Lanthanum Monosulfide (ideal gas)
[Formation: $\text{La}(c) + \text{S}(c,1) = \text{LaS}(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15*	8.220	59.900	59.900	0	32.500	20.980	-15.378
300	8.230	59.950	59.900	.015	32.493	20.908	-15.232
368.3	8.428	61.660	60.071	.585	32.235	18.297	-10.857
368.3	8.428	61.660	60.071	.585	32.139	18.297	-10.857
388.36	8.486	62.109	60.165	.755	32.058	17.546	-9.874
388.36	8.486	62.109	60.165	.755	31.645	17.546	-9.874
400	8.520	62.360	60.225	.854	31.580	17.124	-9.356
432.02	8.562	63.018	60.408	1.127	31.380	15.973	-8.081
500	8.650	64.280	60.854	1.713	30.845	13.594	-5.942
550	8.685	65.103	61.199	2.147	30.513	11.888	-4.724
550	8.685	65.103	61.199	2.147	30.426	11.888	-4.724
600	8.720	65.860	61.557	2.582	30.111	10.216	-3.721
700	8.770	67.210	62.271	3.457	29.508	6.951	-2.170
717.824	8.775	67.431	62.397	3.613	29.403	6.379	-1.942

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
550 K, $\alpha - \beta$ transition point of La; $\Delta H^\circ = 0.087$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2500 K: $C_p^\circ = 8.859 + 0.042 \times 10^{-3}T - 0.579 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 8.859 \times 10^{-3}T + 0.021 \times 10^{-6}T^2 + 0.579 \times 10^{-2}T^{-1} - 2.837$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 34.477 - 5.900 \times 10^{-3}T + 1.688 \times 10^{-6}T^2 - 109.700T^{-1}$
 $\Delta G_f^\circ = 34.477 + 5.900 \times 10^{-3}T \ln T - 1.688 \times 10^{-6}T^2 - 54.850T^{-1} - 77.765 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = 33.362 - 3.637 \times 10^{-3}T - 0.058 \times 10^{-6}T^2 + 45.900T^{-1}$
 $\Delta G_f^\circ = 33.362 + 3.637 \times 10^{-3}T \ln T + 0.058 \times 10^{-6}T^2 + 22.950T^{-1} - 62.582 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = 17.204 + 41.103 \times 10^{-3}T - 43.340 \times 10^{-6}T^2 + 1948.100T^{-1}$
 $\Delta G_f^\circ = 17.204 - 41.103 \times 10^{-3}T \ln T + 43.340 \times 10^{-6}T^2 + 974.050T^{-1} + 222.646 \times 10^{-3}T$
432.02-550 K: $\Delta H_f^\circ = 7.725 + 37.197 \times 10^{-3}T - 23.528 \times 10^{-6}T^2 + 5174.600T^{-1}$
 $\Delta G_f^\circ = 7.725 - 37.197 \times 10^{-3}T \ln T + 23.528 \times 10^{-6}T^2 + 2587.300T^{-1} + 220.799 \times 10^{-3}T$
550-717.824 K: $\Delta H_f^\circ = 6.745 + 39.463 \times 10^{-3}T - 25.230 \times 10^{-6}T^2 + 5263.400T^{-1}$
 $\Delta G_f^\circ = 6.745 - 39.463 \times 10^{-3}T \ln T + 25.230 \times 10^{-6}T^2 + 2631.700T^{-1} + 235.796 \times 10^{-3}T$

LaS(g)
Lanthanum Monosulfide (ideal gas)
[Reaction: $\text{La(c,l)} + 0.5\text{S}_2(\text{g}) = \text{LaS(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔH°	ΔG°	
298.15*	8.220	59.900	59.900	0	17.145	11.466	-8.405
300	8.230	59.950	59.900	.015	17.141	11.431	-8.328
400	8.520	62.360	60.225	.854	16.929	9.558	-5.222
500	8.650	64.280	60.854	1.713	16.718	7.740	-3.383
550	8.685	65.103	61.199	2.147	16.610	6.850	-2.722
550	8.685	65.103	61.199	2.147	16.523	6.850	-2.722
600	8.720	65.860	61.557	2.582	16.417	5.975	-2.176
700	8.770	67.210	62.271	3.457	16.183	4.256	-1.329
800	8.800	68.390	62.970	4.336	15.918	2.561	-.700
900	8.820	69.420	63.623	5.217	15.619	.914	-.222
1000	8.840	70.350	64.249	6.101	15.287	-.694	.152
1100	8.860	71.200	64.849	6.986	14.917	-2.281	.453
1134	8.863	71.470	65.044	7.287	14.784	-2.812	.542
1134	8.863	71.470	65.044	7.287	14.038	-2.812	.542
1193	8.869	71.918	65.372	7.810	13.735	-3.680	.674
1193	8.869	71.918	65.372	7.810	12.254	-3.680	.674
1200	8.870	71.970	65.410	7.872	12.228	-3.771	.687
1300	8.880	72.680	65.942	8.760	11.841	-5.097	.857
1400	8.890	73.340	66.449	9.648	11.450	-6.384	.997
1500	8.900	73.950	66.925	10.537	11.057	-7.633	1.112
1600	8.900	74.530	67.388	11.427	10.662	-8.874	1.212
1700	8.910	75.070	67.824	12.318	10.264	-10.095	1.298
1800	8.920	75.580	68.242	13.209	9.862	-11.279	1.369
1900	8.920	76.060	68.638	14.101	9.459	-12.426	1.429
2000	8.930	76.520	69.023	14.994	9.053	-13.572	1.483

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 550 K, $\alpha - \beta$ transition point of La; $\Delta\text{H}^\circ = 0.087$ kcal/mol.
1134 K, $\beta - \gamma$ transition point of La; $\Delta\text{H}^\circ = 0.746$ kcal/mol.
1193 K, melting point of La; $\Delta\text{H}^\circ = 1.481$ kcal/mol.

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

298.15-2500 K: $\text{Cp}^\circ = 8.859 + 0.042 \times 10^{-3}\text{T} - 0.579 \times 10^{-5}\text{T}^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 8.859 \times 10^{-3}\text{T} + 0.021 \times 10^{-6}\text{T}^2 + 0.579 \times 10^{-2}\text{T}^{-1} - 2.837$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta\text{H}^\circ = 17.688 - 1.897 \times 10^{-3}\text{T} - 0.189 \times 10^{-6}\text{T}^2 + 11.750\text{T}^{-1}$
 $\Delta\text{G}^\circ = 17.688 + 1.897 \times 10^{-3}\text{T} \ln \text{T} + 0.189 \times 10^{-6}\text{T}^2 + 5.875\text{T}^{-1} - 31.802 \times 10^{-3}\text{T}$
550-1134 K: $\Delta\text{H}^\circ = 16.708 + 0.369 \times 10^{-3}\text{T} - 1.891 \times 10^{-6}\text{T}^2 + 100.550\text{T}^{-1}$
 $\Delta\text{G}^\circ = 16.708 - 0.369 \times 10^{-3}\text{T} \ln \text{T} + 1.891 \times 10^{-6}\text{T}^2 + 50.275\text{T}^{-1} - 16.805 \times 10^{-3}\text{T}$
1134-1193 K: $\Delta\text{H}^\circ = 19.624 - 4.787 \times 10^{-3}\text{T} - 0.139 \times 10^{-6}\text{T}^2 + 23.750\text{T}^{-1}$
 $\Delta\text{G}^\circ = 19.624 + 4.787 \times 10^{-3}\text{T} \ln \text{T} + 0.139 \times 10^{-6}\text{T}^2 + 11.875\text{T}^{-1} - 53.625 \times 10^{-3}\text{T}$
1193-2000 K: $\Delta\text{H}^\circ = 16.622 - 3.512 \times 10^{-3}\text{T} - 0.139 \times 10^{-6}\text{T}^2 + 23.750\text{T}^{-1}$
 $\Delta\text{G}^\circ = 16.622 + 3.512 \times 10^{-3}\text{T} \ln \text{T} + 0.139 \times 10^{-6}\text{T}^2 + 11.875\text{T}^{-1} - 42.076 \times 10^{-3}\text{T}$

Sources: Enthalpy of formation at 298 K from Schumm (104). Other data are those estimated by Mills (80).

La₂S₃(c)
Dilanthanum Trisulfide
[Formation: 2La(c) + 3S(c,l) = La₂S₃(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	28.890	39.430	39.430	0	-289.000	-285.794	209.490
300*	28.930	39.610	39.433	.053	-289.001	-285.774	208.184
368.3	29.927	45.660	40.037	2.071	-289.024	-285.040	169.141
368.3	29.927	45.660	40.037	2.071	-289.312	-285.040	169.141
388.36	30.220	47.255	40.369	2.674	-289.328	-284.805	160.272
388.36	30.220	47.255	40.369	2.674	-290.567	-284.805	160.272
400	30.390	48.150	40.583	3.027	-290.631	-284.632	155.514
432.02	30.656	50.500	41.232	4.004	-290.863	-284.145	143.741
500	31.220	55.030	42.808	6.111	-291.672	-283.011	123.703
550	31.510	58.026	44.062	7.680	-292.071	-282.124	112.104
550	31.510	58.026	44.062	7.680	-292.245	-282.124	112.104
600	31.800	60.780	45.342	9.263	-292.583	-281.191	102.423
700	32.260	65.710	47.901	12.466	-293.136	-279.235	87.180
717.824	32.333	66.522	48.354	13.042	-293.219	-278.879	84.907

*Data above 298 K estimated.

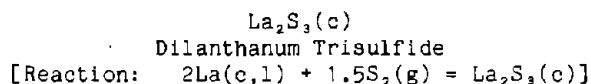
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
550 K, α - β transition point of La; ΔH° = 0.087 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 30.621 + 3.034x10⁻³T - 2.343x10⁻⁵T⁻²
H°- H₂₉₈° = 30.621x10⁻³T + 1.517x10⁻⁶T² + 2.343x10⁻²T⁻¹ - 10.050

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -286.615 - 7.071x10⁻³T + 6.568x10⁻⁶T² - 256.500T⁻¹
ΔGf° = -286.615 + 7.071x10⁻³TlnT - 6.568x10⁻⁶T² - 128.250T⁻¹ - 34.132x10⁻³T
368.3-388.36 K: ΔHf° = -289.961 - 0.282x10⁻³T + 1.330x10⁻⁶T² + 210.300T⁻¹
ΔGf° = -289.961 + 0.282x10⁻³TlnT - 1.330x10⁻⁶T² + 105.150T⁻¹ + 11.417x10⁻³T
388.36-432.02 K: ΔHf° = -338.436 + 133.938x10⁻³T - 128.516x10⁻⁶T² + 5916.900T⁻¹
ΔGf° = -338.436 - 133.938x10⁻³TlnT + 128.516x10⁻⁶T² + 2958.450T⁻¹ + 867.102x10⁻³T
432.02-550 K: ΔHf° = -366.872 + 122.220x10⁻³T - 69.080x10⁻⁶T² + 15596.400T⁻¹
ΔGf° = -366.872 - 122.220x10⁻³TlnT + 69.080x10⁻⁶T² + 7798.200T⁻¹ + 861.560x10⁻³T
550-717.824 K: ΔHf° = -368.831 + 126.752x10⁻³T - 72.484x10⁻⁶T² + 15774.000T⁻¹
ΔGf° = -368.831 - 126.752x10⁻³TlnT + 72.484x10⁻⁶T² + 7887.000T⁻¹ + 891.554x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHr°	ΔGr°	
298.15	28.890	39.430	39.430	0	-335.065	-314.335	230.411
300*	28.930	39.610	39.433	.053	-335.057	-314.206	228.896
400	30.390	48.150	40.583	3.027	-334.584	-307.329	167.915
500	31.220	55.030	42.808	6.111	-334.055	-300.571	131.378
550	31.510	58.026	44.062	7.680	-333.779	-297.237	118.110
550	31.510	58.026	44.062	7.680	-333.953	-297.237	118.110
600	31.800	60.780	45.342	9.263	-333.667	-293.914	107.057
700	32.260	65.710	47.901	12.466	-333.111	-287.321	89.704
800	32.670	70.050	50.409	15.713	-332.586	-280.826	76.717
900	33.040	73.920	52.810	18.999	-332.100	-274.390	66.630
1000	33.400	77.420	55.098	22.322	-331.654	-267.989	58.568
1100	33.740	80.620	57.275	25.679	-331.254	-261.640	51.982
1134	33.856	81.649	57.991	26.828	-331.127	-259.494	50.010
1134	33.856	81.649	57.991	26.828	-332.619	-259.494	50.010
1193	34.056	83.371	59.203	28.832	-332.533	-255.690	46.840
1193	34.056	83.371	59.203	28.832	-335.495	-255.690	46.840
1200	34.080	83.570	59.345	29.070	-335.465	-255.218	46.481
1300	34.410	86.310	61.315	32.494	-335.045	-248.565	41.787
1400	34.740	88.870	63.190	35.952	-334.603	-241.918	37.765
1500	35.070	91.280	64.985	39.442	-334.139	-235.306	34.284
1600	35.400	93.550	66.696	42.966	-333.651	-228.723	31.242
1700	35.730	95.710	68.344	46.523	-333.143	-222.212	28.567
1800	36.070	97.760	69.919	50.113	-332.609	-215.692	26.188
1900	36.400	99.720	71.437	53.737	-332.051	-209.188	24.062
2000	36.740	101.600	72.903	57.394	-331.470	-202.747	22.155

*Data above 298 K estimated.

Phase changes: 550 K, $\alpha - \beta$ transition point of La; $\Delta\text{H}^\circ = 0.087$ kcal/mol.
 1134 K, $\beta - \gamma$ transition point of La; $\Delta\text{H}^\circ = 0.746$ kcal/mol.
 1193 K, melting point of La; $\Delta\text{H}^\circ = 1.481$ kcal/mol.

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

298.15-2000 K: $\text{Cp}^\circ = 30.621 + 3.034 \times 10^{-3}\text{T} - 2.343 \times 10^{-5}\text{T}^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 30.621 \times 10^{-3}\text{T} + 1.517 \times 10^{-6}\text{T}^2 + 2.343 \times 10^{-2}\text{T}^3 - 10.050$

Reaction equations (kcal/mol):

298.15-550 K: $\Delta\text{Hr}^\circ = -336.982 + 4.936 \times 10^{-3}\text{T} + 0.937 \times 10^{-6}\text{T}^2 + 107.850\text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -336.982 - 4.936 \times 10^{-3}\text{T} \ln \text{T} - 0.937 \times 10^{-6}\text{T}^2 + 53.925\text{T}^{-1} + 103.757 \times 10^{-3}\text{T}$
 550-1134 K: $\Delta\text{Hr}^\circ = -338.942 + 9.468 \times 10^{-3}\text{T} - 2.467 \times 10^{-6}\text{T}^2 + 285.450\text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -338.942 - 9.468 \times 10^{-3}\text{T} \ln \text{T} + 2.467 \times 10^{-6}\text{T}^2 + 142.725\text{T}^{-1} + 133.751 \times 10^{-3}\text{T}$
 1134-1193 K: $\Delta\text{Hr}^\circ = -333.110 - 0.844 \times 10^{-3}\text{T} + 1.037 \times 10^{-6}\text{T}^2 + 131.850\text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -333.110 + 0.844 \times 10^{-3}\text{T} \ln \text{T} - 1.037 \times 10^{-6}\text{T}^2 + 65.925\text{T}^{-1} + 60.112 \times 10^{-3}\text{T}$
 1193-2000 K: $\Delta\text{Hr}^\circ = -339.114 + 1.706 \times 10^{-3}\text{T} + 1.037 \times 10^{-6}\text{T}^2 + 131.850\text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -339.114 - 1.706 \times 10^{-3}\text{T} \ln \text{T} - 1.037 \times 10^{-6}\text{T}^2 + 65.925\text{T}^{-1} + 83.210 \times 10^{-3}\text{T}$

Sources: Enthalpy of formation at 298 K from Schumm (104). Low-temperature heat capacities and entropy at 298 K from Paukov (96). Data above 298 K estimated.

LuS(g)
Lutetium Monosulfide (ideal gas)
[Formation: $\text{Lu(c)} + \text{S(c,l)} = \text{LuS(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	8.200	60.520	60.520	0	47.500	35.372	-25.928
300	8.210	60.570	60.520	.015	47.493	35.297	-25.713
368.3	8.415	62.281	60.694	.585	47.241	32.544	-19.311
368.3	8.415	62.281	60.694	.585	47.145	32.544	-19.311
388.36	8.475	62.729	60.787	.754	47.067	31.752	-17.868
388.36	8.475	62.729	60.787	.754	46.654	31.752	-17.868
400	8.510	62.980	60.847	.853	46.590	31.306	-17.104
432.02	8.555	63.637	61.030	1.126	46.394	30.089	-15.221
500	8.650	64.890	61.466	1.712	45.868	27.572	-12.051
600	8.730	66.480	62.178	2.581	45.232	23.969	-8.731
700	8.780	67.830	62.893	3.456	44.653	20.472	-6.392
717.824	8.785	68.051	63.018	3.613	44.554	19.858	-6.046

*Data except enthalpy of formation at 298 K estimated.

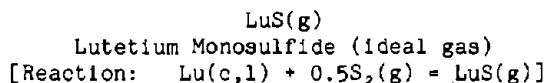
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $C_p^\circ = 8.875 + 0.036 \times 10^{-3}T - 0.608 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 8.875 \times 10^{-3}T + 0.018 \times 10^{-6}T^2 + 0.608 \times 10^{-2}T^{-1} - 2.852$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 48.338 - 3.196 \times 10^{-3}T - 0.019 \times 10^{-6}T^2 + 34.700T^{-1}$
 $\Delta G_f^\circ = 48.338 + 3.196 \times 10^{-3}T \ln T + 0.019 \times 10^{-6}T^2 + 17.350T^{-1} - 61.901 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = 47.223 - 0.933 \times 10^{-3}T - 1.765 \times 10^{-6}T^2 + 190.300T^{-1}$
 $\Delta G_f^\circ = 47.223 + 0.933 \times 10^{-3}T \ln T + 1.765 \times 10^{-6}T^2 + 95.150T^{-1} - 46.718 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = 31.065 + 43.807 \times 10^{-3}T - 45.047 \times 10^{-6}T^2 + 2092.500T^{-1}$
 $\Delta G_f^\circ = 31.065 - 43.807 \times 10^{-3}T \ln T + 45.047 \times 10^{-6}T^2 + 1046.250T^{-1} + 238.511 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = 21.586 + 39.901 \times 10^{-3}T - 25.235 \times 10^{-6}T^2 + 5319.000T^{-1}$
 $\Delta G_f^\circ = 21.586 - 39.901 \times 10^{-3}T \ln T + 25.235 \times 10^{-6}T^2 + 2659.500T^{-1} + 236.663 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15*	8.200	60.520	60.520	0	32.145	25.858	-18.954
300	8.210	60.570	60.520	.015	32.141	25.819	-18.809
400	8.510	62.980	60.847	.853	31.939	23.740	-12.971
500	8.650	64.890	61.466	1.712	31.741	21.718	-9.493
600	8.730	66.480	62.178	2.581	31.538	19.728	-7.186
700	8.780	67.830	62.893	3.456	31.328	17.777	-5.550
800	8.810	69.000	63.581	4.335	31.101	15.864	-4.334
900	8.830	70.040	64.243	5.217	30.854	13.971	-3.393
1000	8.850	70.970	64.868	6.102	30.584	12.113	-2.647
1100	8.860	71.820	65.468	6.987	30.283	10.269	-2.040
1200	8.880	72.590	66.028	7.874	29.951	8.469	-1.542
1300	8.880	73.300	66.560	8.762	29.581	6.689	-1.125
1400	8.890	73.960	67.066	9.651	29.170	4.951	-.773
1500	8.900	74.570	67.543	10.541	28.712	3.242	-.472
1600	8.910	75.150	68.005	11.432	28.205	1.549	-.212
1700	8.910	75.690	68.441	12.323	27.644	-.110	.014
1800	8.920	76.200	68.859	13.214	27.022	-1.715	.208
1900	8.930	76.680	69.255	14.107	26.342	-3.295	.379
1936	8.930	76.848	69.395	14.428	26.084	-3.862	.436
1936	8.930	76.848	69.395	14.428	21.627	-3.862	.436
2000	8.930	77.140	69.640	15.000	21.162	-4.683	.512

*Data except enthalpy of formation at 298 K estimated.

Phase change: 1936 K, melting point of Lu; ΔH° = 4.457 kcal/mol.

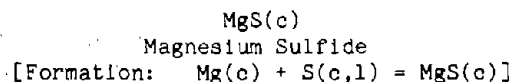
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 8.875 + 0.036 \times 10^{-3}T - 0.608 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 8.875 \times 10^{-3}T + 0.018 \times 10^{-6}T^2 + 0.608 \times 10^{-2}T^{-1} - 2.852$

Reaction equations (kcal/mol):

298.15-1936 K: $\Delta H_r^\circ = 31.549 + 0.807 \times 10^{-3}T - 1.896 \times 10^{-6}T^2 + 156.150T^{-1}$
 $\Delta G_r^\circ = 31.549 - 0.807 \times 10^{-3}T \ln T + 1.896 \times 10^{-6}T^2 + 78.075T^{-1} - 15.938 \times 10^{-3}T$
 1936-2000 K: $\Delta H_r^\circ = 35.208 - 6.747 \times 10^{-3}T - 0.142 \times 10^{-6}T^2 + 26.650T^{-1}$
 $\Delta G_r^\circ = 35.208 + 6.747 \times 10^{-3}T \ln T + 0.142 \times 10^{-6}T^2 + 13.325T^{-1} - 71.578 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Franzen (41). Other data are those estimated by Mills (80).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°-H ₂₉₈ °)/T	H°-H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	10.890	12.030	12.030	0	-82.630	-81.604	59.817
300	10.910	12.097	12.030	.020	-82.631	-81.597	59.442
368.3*	11.231	14.371	12.259	.778	-82.671	-81.359	48.278
368.3	11.231	14.371	12.259	.778	-82.767	-81.359	48.278
388.36	11.325	14.969	12.384	1.004	-82.784	-81.281	45.740
388.36	11.325	14.969	12.384	1.004	-83.197	-81.281	45.740
400	11.380	15.304	12.464	1.136	-83.225	-81.223	44.378
432.02	11.482	16.184	12.708	1.502	-83.323	-81.060	41.006
500	11.700	17.879	13.297	2.291	-83.646	-80.677	35.263
600	11.930	20.034	14.246	3.473	-83.987	-80.046	29.156
700	12.080	21.885	15.208	4.674	-84.280	-79.365	24.779
717.824	12.100	22.189	15.377	4.889	-84.328	-79.239	24.125

*Data above 320 K estimated.

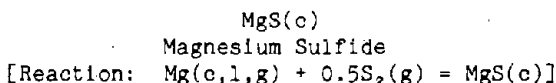
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2500 K: $\text{Cp}^\circ = 11.579 + 0.922 \times 10^{-3}T - 0.856 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 11.579 \times 10^{-3}T + 0.461 \times 10^{-6}T^2 + 0.856 \times 10^{-2}T^{-1} - 3.780$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta \text{Hf}^\circ = -81.941 - 1.738 \times 10^{-3}T + 0.790 \times 10^{-6}T^2 - 71.900T^{-1}$
 $\Delta \text{Gf}^\circ = -81.941 + 1.738 \times 10^{-3}T \ln T - 0.790 \times 10^{-6}T^2 - 35.950T^{-1} - 8.133 \times 10^{-3}T$
 368.3-388.36 K: $\Delta \text{Hf}^\circ = -83.056 + 0.525 \times 10^{-3}T - 0.956 \times 10^{-6}T^2 + 83.700T^{-1}$
 $\Delta \text{Gf}^\circ = -83.056 - 0.525 \times 10^{-3}T \ln T + 0.956 \times 10^{-6}T^2 + 41.850T^{-1} + 7.050 \times 10^{-3}T$
 388.36-432.02 K: $\Delta \text{Hf}^\circ = -99.214 + 45.265 \times 10^{-3}T - 44.238 \times 10^{-6}T^2 + 1985.900T^{-1}$
 $\Delta \text{Gf}^\circ = -99.214 - 45.265 \times 10^{-3}T \ln T + 44.238 \times 10^{-6}T^2 + 992.950T^{-1} + 292.279 \times 10^{-3}T$
 432.02-717.824 K: $\Delta \text{Hf}^\circ = -108.693 + 41.359 \times 10^{-3}T - 24.426 \times 10^{-6}T^2 + 5212.400T^{-1}$
 $\Delta \text{Gf}^\circ = -108.693 - 41.359 \times 10^{-3}T \ln T + 24.426 \times 10^{-6}T^2 + 2606.200T^{-1} + 290.431 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	10.890	12.030	12.030	0	-97.985	-91.118	66.790
300	10.910	12.097	12.030	.020	-97.983	-91.074	66.346
400*	11.380	15.304	12.464	1.136	-97.876	-88.789	48.511
500	11.700	17.879	13.297	2.291	-97.773	-86.530	37.822
600	11.930	20.034	14.246	3.473	-97.681	-84.287	30.701
700	12.080	21.885	15.208	4.674	-97.605	-82.060	25.620
800	12.190	23.505	16.146	5.887	-97.549	-79.847	21.813
900	12.300	24.947	17.045	7.112	-97.515	-77.631	18.851
922	12.322	25.244	17.237	7.383	-97.510	-77.149	18.287
922	12.322	25.244	17.237	7.383	-99.649	-77.149	18.287
1000	12.400	26.248	17.901	8.347	-99.641	-75.250	16.446
1100	12.511	27.436	18.716	9.592	-99.643	-72.816	14.467
1200	12.620	28.529	19.488	10.849	-99.668	-70.377	12.817
1300	12.727	29.543	20.223	12.116	-99.705	-67.923	11.419
1363	12.792	30.147	20.668	12.920	-99.739	-66.401	10.647
1363	12.792	30.147	20.668	12.920	-129.989	-66.401	10.647
1400	12.830	30.490	20.923	13.394	-129.870	-64.677	10.096
1500	12.924	31.379	21.591	14.682	-129.540	-60.034	8.747
1600	13.020	32.216	22.229	15.979	-129.206	-55.411	7.569
1700	13.124	33.008	22.840	17.286	-128.866	-50.809	6.532
1800	13.220	33.761	23.425	18.604	-128.516	-46.226	5.613
1900	13.300	34.478	23.989	19.929	-128.163	-41.665	4.792
2000	13.390	35.162	24.530	21.264	-127.803	-37.119	4.056

*Data above 320 K estimated.

Phase changes: 922 K, melting point of Mg; $\Delta H^\circ = 2.139$ kcal/mol.
1363 K, boiling point of Mg; $\Delta H^\circ = 30.250$ kcal/mol.

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

298.15-2500 K: $C_p^\circ = 11.579 + 0.922 \times 10^{-3}T - 0.856 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 11.579 \times 10^{-3}T + 0.461 \times 10^{-6}T^2 + 0.856 \times 10^{-2}T^{-1} - 3.780$

Reaction equations (kcal/mol):

298.15-922 K: $\Delta H_r^\circ = -98.730 + 2.264 \times 10^{-3}T - 1.087 \times 10^{-6}T^2 + 49.550T^{-1}$
 $\Delta G_r^\circ = -98.730 - 2.264 \times 10^{-3}T \ln T + 1.087 \times 10^{-6}T^2 + 24.775T^{-1} + 37.830 \times 10^{-3}T$
922-1363 K: $\Delta H_r^\circ = -100.053 + 1.399 \times 10^{-3}T - 0.773 \times 10^{-6}T^2 - 212.150T^{-1}$
 $\Delta G_r^\circ = -100.053 - 1.399 \times 10^{-3}T \ln T + 0.773 \times 10^{-6}T^2 - 106.075T^{-1} + 33.798 \times 10^{-3}T$
1363-2000 K: $\Delta H_r^\circ = -133.911 + 2.439 \times 10^{-3}T + 0.301 \times 10^{-6}T^2 + 51.450T^{-1}$
 $\Delta G_r^\circ = -133.911 - 2.439 \times 10^{-3}T \ln T - 0.301 \times 10^{-6}T^2 + 25.725T^{-1} + 67.544 \times 10^{-3}T$

Source: Data from Chase (17) who estimated all above 320 K.

MgS(g)
Magnesium Sulfide (ideal gas)
[Formation: $\text{Mg(c)} + \text{S(c,l)} = \text{MgS(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	8.269	53.866	53.866	0	34.710	23.263	-17.052
300	8.281	53.917	53.867	.015	34.704	23.192	-16.895
368.3	8.823	55.660	54.041	.596	34.488	20.593	-12.220
368.3	8.823	55.660	54.041	.596	34.392	20.593	-12.220
388.36	8.983	56.132	54.137	.775	34.327	19.844	-11.167
388.36	8.983	56.132	54.137	.775	33.914	19.844	-11.167
400	9.075	56.399	54.199	.880	33.859	19.423	-10.612
432.02	9.454	57.112	54.389	1.177	33.691	18.273	-9.244
500	10.259	58.545	54.857	1.844	33.247	15.883	-6.942
600	11.567	60.533	55.640	2.936	32.816	12.457	-4.538
700	12.605	62.399	56.473	4.148	32.534	9.089	-2.838
717.824	12.706	62.717	56.624	4.374	32.496	8.493	-2.586

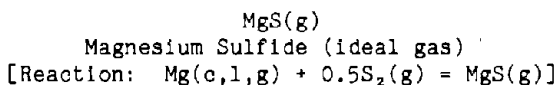
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2500 K: $C_p^\circ = 13.623 - 1.210 \times 10^{-3}T + 4.439 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 13.623 \times 10^{-3}T - 0.605 \times 10^{-6}T^2 + 4.439 \times 10^{-2}T^3 - 5.497$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 33.683 + 0.306 \times 10^{-3}T - 0.276 \times 10^{-6}T^2 + 286.400T^{-1}$
 $\Delta G_f^\circ = 33.683 - 0.306 \times 10^{-3}T \ln T + 0.276 \times 10^{-6}T^2 + 143.200T^{-1} - 34.899 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = 32.568 + 2.569 \times 10^{-3}T - 2.022 \times 10^{-6}T^2 + 442.000T^{-1}$
 $\Delta G_f^\circ = 32.568 - 2.569 \times 10^{-3}T \ln T + 2.022 \times 10^{-6}T^2 + 221.000T^{-1} - 19.716 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = 16.409 + 47.309 \times 10^{-3}T - 45.304 \times 10^{-6}T^2 + 2344.200T^{-1}$
 $\Delta G_f^\circ = 16.409 - 47.309 \times 10^{-3}T \ln T + 45.304 \times 10^{-6}T^2 + 1172.100T^{-1} + 265.512 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = 6.931 + 43.403 \times 10^{-3}T - 25.492 \times 10^{-6}T^2 + 5570.700T^{-1}$
 $\Delta G_f^\circ = 6.931 - 43.403 \times 10^{-3}T \ln T + 25.492 \times 10^{-6}T^2 + 2785.350T^{-1} + 263.665 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15	8.269	53.866	53.866	0	19.355	13.749	-10.078
300	8.281	53.917	53.867	.015	19.352	13.715	-9.991
400	9.075	56.399	54.199	.880	19.208	11.857	-6.478
500	10.259	58.545	54.857	1.844	19.120	10.030	-4.384
600	11.567	60.533	55.640	2.936	19.122	8.217	-2.993
700	12.605	62.399	56.473	4.148	19.209	6.394	-1.996
800	13.169	64.125	57.324	5.441	19.344	4.551	-1.243
900	13.287	65.686	58.167	6.767	19.480	2.699	-.655
922	13.246	66.006	58.350	7.059	19.506	2.284	-.541
922	13.246	66.006	58.350	7.059	17.367	2.284	-.541
1000	13.102	67.078	58.990	8.088	17.440	1.000	-.219
1100	12.758	68.312	59.783	9.382	17.486	-.649	.129
1200	12.361	69.405	60.540	10.638	17.461	-2.300	.419
1300	11.969	70.379	61.260	11.855	17.374	-3.930	.661
1363	11.744	70.940	61.695	12.601	17.281	-4.981	.799
1363	11.744	70.940	61.695	12.601	-12.969	-4.981	.799
1400	11.612	71.253	61.944	13.033	-12.890	-4.766	.744
1500	11.300	72.043	62.591	14.178	-12.705	-4.194	.611
1600	11.033	72.763	63.204	15.295	-12.550	-3.630	.496
1700	10.807	73.425	63.786	16.386	-12.425	-3.078	.396
1800	10.618	74.037	64.339	17.457	-12.323	-2.530	.307
1900	10.460	74.607	64.864	18.511	-12.241	-1.988	.229
2000	10.328	75.140	65.365	19.550	-12.178	-1.449	.158

Phase changes: 922 K, melting point of Mg; $\Delta H^\circ = 2.139$ kcal/mol.
1363 K, boiling point of Mg; $\Delta H^\circ = 30.250$ kcal/mol.

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

298.15-2500 K: $C_p^\circ = 13.623 - 1.210 \times 10^{-3}T - 4.439 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 13.623 \times 10^{-3}T - 0.605 \times 10^{-5}T^2 + 4.439 \times 10^{-2}T^{-1} - 5.497$

Reaction equations (kcal/mol):

298.15-922 K: $\Delta H_r^\circ = 16.894 + 4.308 \times 10^{-3}T - 2.153 \times 10^{-6}T^2 + 407.850T^{-1}$
 $\Delta G_r^\circ = 16.894 - 4.308 \times 10^{-3}T \ln T + 2.153 \times 10^{-6}T^2 + 203.925T^{-1} + 11.064 \times 10^{-3}T$
922-1363 K: $\Delta H_r^\circ = 15.570 + 3.442 \times 10^{-3}T - 1.839 \times 10^{-6}T^2 + 146.150T^{-1}$
 $\Delta G_r^\circ = 15.570 - 3.442 \times 10^{-3}T \ln T + 1.839 \times 10^{-6}T^2 + 73.075T^{-1} + 7.031 \times 10^{-3}T$
1363-2000 K: $\Delta H_r^\circ = -18.287 + 4.483 \times 10^{-3}T - 0.765 \times 10^{-6}T^2 + 409.750T^{-1}$
 $\Delta G_r^\circ = -18.287 - 4.483 \times 10^{-3}T \ln T + 0.765 \times 10^{-6}T^2 + 204.875T^{-1} + 40.778 \times 10^{-3}T$

Source: Data from Chase (17) who estimated some molecular constants.

MnS(c)
Manganese Monosulfide
[Formation: $\text{Mn(c)} + \text{S(c,l)} = \text{MnS(c)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	11.940	19.200	19.200	0	-51.200	-52.360	38.380
300	11.956	19.274	19.201	.022	-51.200	-52.367	38.149
368.3	12.278	21.770	19.453	.853	-51.193	-52.635	31.233
368.3	12.278	21.770	19.453	.853	-51.289	-52.635	31.233
388.36	12.373	22.424	19.590	1.101	-51.294	-52.707	29.661
388.36	12.373	22.424	19.590	1.101	-51.707	-52.707	29.661
400	12.428	22.790	19.678	1.245	-51.729	-52.737	28.814
432.02	12.474	23.749	19.944	1.644	-51.812	-52.816	26.718
500	12.571	25.582	20.588	2.497	-52.112	-52.944	23.142
600	12.613	27.878	21.618	3.756	-52.452	-53.080	19.334
700	12.637	29.824	22.654	5.019	-52.771	-53.162	16.598
717.824	12.644	30.142	22.836	5.244	-52.826	-53.170	16.188

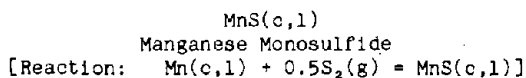
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1803 K: $C_p^\circ = 11.159 + 2.046 \times 10^{-3}T + 0.152 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 11.159 \times 10^{-3}T + 1.023 \times 10^{-6}T^2 - 0.152 \times 10^{-2}T^{-1} - 3.367$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -49.816 - 2.653 \times 10^{-3}T + 1.033 \times 10^{-6}T^2 - 204.200T^{-1}$
 $\Delta G_f^\circ = -49.816 + 2.653 \times 10^{-3}T \ln T - 1.033 \times 10^{-6}T^2 - 102.100T^{-1} - 22.190 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -50.931 - 0.390 \times 10^{-3}T - 0.713 \times 10^{-6}T^2 - 48.600T^{-1}$
 $\Delta G_f^\circ = -50.931 + 0.390 \times 10^{-3}T \ln T + 0.713 \times 10^{-6}T^2 - 24.300T^{-1} - 7.007 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -67.089 + 44.350 \times 10^{-3}T - 43.995 \times 10^{-6}T^2 + 1853.600T^{-1}$
 $\Delta G_f^\circ = -67.089 - 44.350 \times 10^{-3}T \ln T + 43.995 \times 10^{-6}T^2 + 926.800T^{-1} + 278.221 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -76.568 + 40.444 \times 10^{-3}T - 24.183 \times 10^{-6}T^2 + 5080.100T^{-1}$
 $\Delta G_f^\circ = -76.568 - 40.444 \times 10^{-3}T \ln T + 24.183 \times 10^{-6}T^2 + 2540.050T^{-1} + 276.374 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	11.940	19.200	19.200	0	-66.555	-61.873	45.354
300	11.956	19.274	19.201	.022	-66.552	-61.844	45.053
400	12.428	22.790	19.678	1.245	-66.380	-60.303	32.948
500	12.571	25.582	20.588	2.497	-66.240	-58.798	25.700
600	12.613	27.878	21.618	3.756	-66.146	-57.320	20.879
700	12.637	29.824	22.654	5.019	-66.096	-55.857	17.439
800	12.679	31.514	23.658	6.285	-66.084	-54.396	14.860
900	12.754	33.011	24.615	7.556	-66.103	-52.935	12.854
980	12.848	34.101	25.346	8.580	-66.133	-51.760	11.543
980	12.848	34.101	25.346	8.580	-66.665	-51.760	11.543
1000	12.871	34.361	25.524	8.837	-66.677	-51.460	11.246
1100	13.036	35.595	26.384	10.132	-66.735	-49.927	9.919
1200	13.251	36.738	27.200	11.445	-66.789	-48.405	8.816
1300	13.518	37.809	27.975	12.784	-66.830	-46.872	7.880
1360	13.711	38.423	28.423	13.600	-66.850	-45.942	7.383
1360	13.711	38.423	28.423	13.600	-67.357	-45.942	7.383
1400	13.839	38.822	28.714	14.151	-67.404	-45.313	7.074
1410	13.877	38.921	28.786	14.290	-67.415	-45.145	6.997
1410	13.877	38.921	28.786	14.290	-67.864	-45.145	6.997
1500	14.214	39.789	29.420	15.553	-67.998	-43.697	6.367
1517	14.287	39.950	29.537	15.795	-68.021	-43.412	6.254
1517	14.287	39.950	29.537	15.795	-70.903	-43.412	6.254
1600	14.644	40.720	30.098	16.996	-71.002	-41.898	5.723
1700	15.129	41.622	30.749	18.484	-71.084	-40.071	5.151
1800	15.670	42.502	31.378	20.023	-71.117	-38.244	4.643
1803	15.687	42.528	31.397	20.070	-71.117	-38.189	4.629
1803*	16.000	45.967	31.397	26.270	-64.917	-38.189	4.629
1900	16.000	46.805	32.162	27.822	-64.893	-36.761	4.228

*Heat capacity of liquid estimated.

Phase changes: 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.
1410 K, γ - δ transition point of Mn; ΔH° = 0.449 kcal/mol.
1517 K, melting point of Mn; ΔH° = 2.882 kcal/mol.
1803 K, melting point of MnS; ΔH° = 6.200 kcal/mol.

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

298.15-1803 K: Cp° = 11.159 + 2.046x10⁻³T + 0.152x10⁻⁵T²
H° - H°₂₉₈ = 11.159x10⁻³T + 1.023x10⁻⁶T² - 0.152x10⁻²T³ - 3.367
1803-1900 K: Cp° = 16.000
H° - H°₂₉₈ = 16.000x10⁻³T - 2.578

Reaction equations (kcal/mol):

298.15-980 K: ΔHr° = -66.605 + 1.349x10⁻³T - 0.844x10⁻⁶T² - 82.750T⁻¹
ΔGr° = -66.605 - 1.349x10⁻³TlnT + 0.844x10⁻⁶T² - 41.375T⁻¹ + 23.773x10⁻³T
980-1360 K: ΔHr° = -66.186 - 0.831x10⁻³T + 0.299x10⁻⁶T² + 4.050T⁻¹
ΔGr° = -66.186 + 0.831x10⁻³TlnT - 0.299x10⁻⁶T² + 2.025T⁻¹ + 9.398x10⁻³T
1360-1410 K: ΔHr° = -66.158 - 0.603x10⁻³T + 0.137x10⁻⁶T² - 49.350T⁻¹
ΔGr° = -66.158 + 0.603x10⁻³TlnT + 0.137x10⁻⁶T² - 24.675T⁻¹ + 10.452x10⁻³T
1410-1517 K: ΔHr° = -65.906 - 1.191x10⁻³T - 0.072x10⁻⁶T² - 49.350T⁻¹
ΔGr° = -65.906 + 1.191x10⁻³TlnT + 0.072x10⁻⁶T² - 24.675T⁻¹ + 6.094x10⁻³T
1517-1803 K: ΔHr° = -66.660 - 4.012x10⁻³T + 0.863x10⁻⁶T² - 49.350T⁻¹
ΔGr° = -66.660 + 4.012x10⁻³TlnT - 0.863x10⁻⁶T² - 24.675T⁻¹ - 12.653x10⁻³T
1803-1900 K: ΔHr° = -65.872 + 0.829x10⁻³T - 0.160x10⁻⁶T² - 34.150T⁻¹
ΔGr° = -65.872 - 0.829x10⁻³TlnT + 0.160x10⁻⁶T² - 17.075T⁻¹ + 21.357x10⁻³T

Sources: Enthalpy of formation at 298 K based on Adami (1). Entropy at 298 K from Mills (80).
Low-temperature heat capacities from Anderson (2). High-temperature data based on
Coughlin (25). Heat capacity of liquid estimated.

MnS(g)
Manganese Monosulfide (ideal gas)
[Formation: $\text{Mn(c)} + \text{S(c,l)} = \text{MnS(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	8.180	57.360	57.360	0	65.000	52.463	-38.456
300	8.190	57.410	57.360	.016	64.994	52.386	-38.163
368.3	8.402	59.112	57.526	.584	64.738	49.542	-29.398
368.3	8.402	59.112	57.526	.584	64.642	49.542	-29.398
388.36	8.464	59.560	57.620	.753	64.559	48.723	-27.419
388.36	8.464	59.560	57.620	.753	64.146	48.723	-27.419
400	8.500	59.810	57.680	.852	64.078	48.262	-26.369
432.02	8.545	60.466	57.863	1.125	63.869	47.003	-23.778
500	8.640	61.730	58.310	1.710	63.301	44.394	-19.405
600	8.720	63.310	59.013	2.578	62.570	40.683	-14.819
700	8.770	64.660	59.727	3.453	61.863	37.087	-11.579
717.824	8.775	64.881	59.852	3.609	61.739	36.459	-11.100

*Data except enthalpy of formation at 298 K estimated.

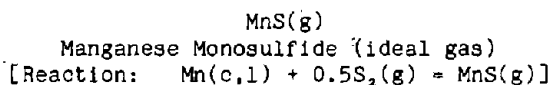
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: $C_p^\circ = 8.877 + 0.032 \times 10^{-3}T - 0.627 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 8.877 \times 10^{-3}T + 0.016 \times 10^{-6}T^2 + 0.627 \times 10^{-2}T^{-1} - 2.858$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 66.893 - 4.935 \times 10^{-3}T + 0.026 \times 10^{-6}T^2 - 126.300T^{-1}$
 $\Delta G_f^\circ = 66.893 + 4.935 \times 10^{-3}T \ln T - 0.026 \times 10^{-6}T^2 - 63.150T^{-1} - 75.797 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = 65.778 - 2.672 \times 10^{-3}T - 1.720 \times 10^{-6}T^2 + 29.300T^{-1}$
 $\Delta G_f^\circ = 65.778 + 2.672 \times 10^{-3}T \ln T + 1.720 \times 10^{-6}T^2 + 14.650T^{-1} - 60.614 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = 49.619 + 42.068 \times 10^{-3}T - 45.002 \times 10^{-6}T^2 + 1931.500T^{-1}$
 $\Delta G_f^\circ = 49.619 - 42.068 \times 10^{-3}T \ln T + 45.002 \times 10^{-6}T^2 + 965.750T^{-1} + 224.615 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = 40.141 + 38.162 \times 10^{-3}T - 25.190 \times 10^{-6}T^2 + 5158.000T^{-1}$
 $\Delta G_f^\circ = 40.141 - 38.162 \times 10^{-3}T \ln T + 25.190 \times 10^{-6}T^2 + 2579.000T^{-1} + 222.767 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15*	8.180	57.360	57.360	0	49.645	42.949	-31.482
300	8.190	57.410	57.360	.016	49.642	42.909	-31.259
400	8.500	59.810	57.680	.852	49.427	40.696	-22.235
500	8.640	61.730	58.310	1.710	49.174	38.541	-16.846
600	8.720	63.310	59.013	2.578	48.876	36.442	-13.274
700	8.770	64.660	59.727	3.453	48.538	34.392	-10.738
800	8.800	65.830	60.415	4.332	48.164	32.398	-8.851
900	8.830	66.870	61.077	5.214	47.755	30.449	-7.394
980	8.846	67.621	61.579	5.921	47.408	28.931	-6.452
980	8.846	67.621	61.579	5.921	46.876	28.931	-6.452
1000	8.850	67.800	61.702	6.098	46.784	28.562	-6.242
1100	8.860	68.650	62.302	6.983	46.317	26.764	-5.317
1200	8.870	69.420	62.862	7.870	45.837	25.002	-4.553
1300	8.880	70.130	63.394	8.757	45.343	23.283	-3.914
1360	8.886	70.532	63.701	9.290	45.041	22.280	-3.580
1360	8.886	70.532	63.701	9.290	44.534	22.280	-3.580
1400	8.890	70.790	63.900	9.646	44.292	21.627	-3.376
1410	8.891	70.853	63.949	9.735	44.230	21.475	-3.329
1410	8.891	70.853	63.949	9.735	43.781	21.475	-3.329
1500	8.900	71.400	64.377	10.535	43.185	20.069	-2.924
1517	8.900	71.500	64.456	10.686	43.070	19.817	-2.855
1517	8.900	71.500	64.456	10.686	40.188	19.817	-2.855
1600	8.900	71.980	64.839	11.425	39.627	18.715	-2.556
1700	8.910	72.520	65.275	12.316	38.949	17.434	-2.241
1800	8.910	73.020	65.683	13.207	38.268	16.208	-1.968
1900	8.920	73.510	66.089	14.099	37.584	14.977	-1.723
2000	8.920	73.960	66.465	14.991	36.897	13.832	-1.511

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 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.
1410 K, γ - δ transition point of Mn; ΔH° = 0.449 kcal/mol.
1517 K, melting point of Mn; ΔH° = 2.882 kcal/mol.

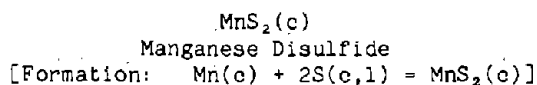
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $\text{Cp}^\circ = 8.877 + 0.032 \times 10^{-3}T - 0.627 \times 10^{-6}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 8.877 \times 10^{-3}T + 0.016 \times 10^{-6}T^2 + 0.627 \times 10^{-2}T^3 - 2.858$

Reaction equations (kcal/mol):

298.15-980 K: $\Delta\text{Hr}^\circ = 50.104 - 0.933 \times 10^{-3}T - 1.851 \times 10^{-6}T^2 - 4.850T^{-1}$
 $\Delta\text{Gr}^\circ = 50.104 + 0.933 \times 10^{-3}T \ln T + 1.851 \times 10^{-6}T^2 - 2.425T^{-1} - 29.834 \times 10^{-3}T$
980-1360 K: $\Delta\text{Hr}^\circ = 50.523 - 3.113 \times 10^{-3}T - 0.708 \times 10^{-6}T^2 + 81.950T^{-1}$
 $\Delta\text{Gr}^\circ = 50.523 + 3.113 \times 10^{-3}T \ln T + 0.708 \times 10^{-6}T^2 + 40.975T^{-1} - 44.208 \times 10^{-3}T$
1360-1410 K: $\Delta\text{Hr}^\circ = 50.550 - 2.885 \times 10^{-3}T - 1.144 \times 10^{-6}T^2 + 28.550T^{-1}$
 $\Delta\text{Gr}^\circ = 50.550 + 2.885 \times 10^{-3}T \ln T + 1.144 \times 10^{-6}T^2 + 14.275T^{-1} - 43.154 \times 10^{-3}T$
1410-1517 K: $\Delta\text{Hr}^\circ = 50.802 - 3.473 \times 10^{-3}T - 1.079 \times 10^{-6}T^2 + 28.550T^{-1}$
 $\Delta\text{Gr}^\circ = 50.802 + 3.473 \times 10^{-3}T \ln T + 1.079 \times 10^{-6}T^2 + 14.275T^{-1} - 47.513 \times 10^{-3}T$
1517-2000 K: $\Delta\text{Hr}^\circ = 50.048 - 6.294 \times 10^{-3}T - 0.144 \times 10^{-6}T^2 + 28.550T^{-1}$
 $\Delta\text{Gr}^\circ = 50.048 + 6.294 \times 10^{-3}T \ln T + 0.144 \times 10^{-6}T^2 + 14.275T^{-1} - 66.259 \times 10^{-3}T$

Source: Data from Mills (80) who estimated all except enthalpy of formation at 298 K.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	16.750	23.880	23.880	0	-53.500	-53.771	39.414
300*	16.770	23.980	23.880	.031	-53.501	-53.771	39.172
368.3	17.405	27.501	24.236	1.203	-53.537	-53.832	31.944
368.3	17.405	27.501	24.236	1.203	-53.729	-53.832	31.944
388.36	17.592	28.429	24.428	1.554	-53.750	-53.836	30.296
388.36	17.592	28.429	24.428	1.554	-54.576	-53.836	30.296
400	17.700	28.950	24.553	1.759	-54.625	-53.814	29.402
432.02	17.911	30.321	24.930	2.329	-54.800	-53.743	27.187
500	18.360	32.970	25.844	3.563	-55.393	-53.521	23.394
600	18.910	36.370	27.325	5.427	-55.985	-53.091	19.338
700	19.400	39.320	28.830	7.343	-56.451	-52.572	16.413

*Data above 298 K estimated.

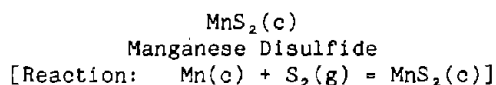
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.

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

298.15-700 K: Cp° = 16.664 + 4.220x10⁻³T - 1.042x10⁻⁵T²
H° - H°₂₉₈ = 16.664x10⁻³T + 2.110x10⁻⁶T² + 1.042x10⁻²T³ - 5.505

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -51.448 - 5.322x10⁻³T + 3.837x10⁻⁶T² - 240.400T⁻¹
ΔGf° = -51.448 + 5.322x10⁻³TlnT - 3.837x10⁻⁶T² - 120.200T⁻¹ - 35.617x10⁻³T
368.3-388.36 K: ΔHf° = -53.678 - 0.796x10⁻³T + 0.345x10⁻⁶T² + 70.800T⁻¹
ΔGf° = -53.678 + 0.796x10⁻³TlnT - 0.345x10⁻⁶T² + 35.400T⁻¹ - 5.251x10⁻³T
388.36-432.02 K: ΔHf° = -85.995 + 88.684x10⁻³T - 86.219x10⁻⁶T² + 3875.200T⁻¹
ΔGf° = -85.995 + 88.684x10⁻³TlnT + 86.219x10⁻⁶T² + 1937.600T⁻¹ + 565.206x10⁻³T
432.02-700 K: ΔHf° = -104.952 + 80.872x10⁻³T - 46.595x10⁻⁶T² + 10328.200T⁻¹
ΔGf° = -104.952 - 80.872x10⁻³TlnT + 46.595x10⁻⁶T² + 5164.100T⁻¹ + 561.511x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈	ΔHr°	ΔGr°	
298.15	16.750	23.880	23.880	0	-84.210	-72.798	53.362
300*	16.770	23.980	23.880	.031	-84.205	-72.726	52.980
400	17.700	28.950	24.553	1.759	-83.927	-68.945	37.669
500	18.360	32.970	25.844	3.563	-83.648	-65.228	28.511
600	18.910	36.370	27.325	5.427	-83.374	-61.572	22.427
700	19.400	39.320	28.830	7.343	-83.101	-57.962	18.096

*Data above 298 K estimated.

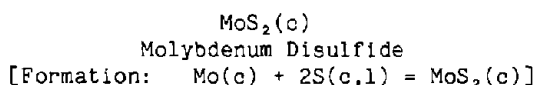
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $C_p^\circ = 16.664 + 4.220 \times 10^{-3}T - 1.042 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 16.664 \times 10^{-3}T + 2.110 \times 10^{-6}T^2 + 1.042 \times 10^{-2}T^{-1} - 5.505$

Reaction equations (kcal/mol):

298.15-700 K: $\Delta H_r^\circ = -85.026 + 2.683 \times 10^{-3}T + 0.083 \times 10^{-6}T^2 + 2.500T^{-1}$
 $\Delta G_r^\circ = -85.026 - 2.683 \times 10^{-3}T \ln T - 0.083 \times 10^{-6}T^2 + 1.250T^{-1} + 56.309 \times 10^{-3}T$

Source: Data from Mills (80) who estimated all above 298 K.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	15.190	14.955	14.955	0	-66.000	-63.848	46.801
300	15.220	15.049	14.956	.028	-66.003	-63.835	46.503
368.3	16.074	18.278	15.278	1.105	-66.092	-63.332	37.581
368.3	16.074	18.278	15.278	1.105	-66.284	-63.332	37.581
388.36	16.324	19.138	15.455	1.430	-66.316	-63.169	35.548
388.36	16.324	19.138	15.455	1.430	-67.142	-63.169	35.548
400	16.470	19.622	15.569	1.621	-67.197	-63.049	34.448
432.02	16.688	20.899	15.918	2.152	-67.385	-62.711	31.724
500	17.150	23.376	16.768	3.304	-67.995	-61.922	27.066
600	17.590	26.543	18.140	5.042	-68.596	-60.648	22.091
700	17.930	29.281	19.541	6.818	-69.057	-59.285	18.509
717.824	17.982	29.732	19.788	7.138	-69.126	-59.034	17.974

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 17.132 + 1.784x10⁻³T - 2.199x10⁻⁵T²
 H° - H°₂₉₈ = 17.132x10⁻³T + 0.892x10⁻⁶T² + 2.199x10⁻²T⁻¹ - 5.925

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -65.100 - 3.593x10⁻³T + 3.141x10⁻⁶T² - 32.100T⁻¹
 ΔGf° = -65.100 + 3.593x10⁻³T ln T - 3.141x10⁻⁶T² - 16.050T⁻¹ - 15.155x10⁻³T
 368.3-388.36 K: ΔHf° = -67.331 + 0.933x10⁻³T - 0.351x10⁻⁶T² + 279.100T⁻¹
 ΔGf° = -67.331 - 0.933x10⁻³T ln T + 0.351x10⁻⁶T² + 139.550T⁻¹ + 15.211x10⁻³T
 388.36-432.02 K: ΔHf° = -99.647 + 90.413x10⁻³T - 86.915x10⁻⁶T² + 4083.500T⁻¹
 ΔGf° = -99.647 - 90.413x10⁻³T ln T + 86.915x10⁻⁶T² + 2041.750T⁻¹ + 585.667x10⁻³T
 432.02-717.824 K: ΔHf° = -118.604 + 82.601x10⁻³T - 47.291x10⁻⁶T² + 10536.500T⁻¹
 ΔGf° = -118.604 - 82.601x10⁻³T ln T + 47.291x10⁻⁶T² + 5268.250T⁻¹ + 581.973x10⁻³T

MoS₂(c)
Molybdenum Disulfide
[Reaction: Mo(c) + S₂(g) = MoS₂(c)]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	15.190	14.955	14.955	0	-96.710	-82.876	60.749
300	15.220	15.049	14.956	.028	-96.707	-82.789	60.311
400	16.470	19.622	15.569	1.621	-96.499	-78.181	42.715
500	17.150	23.376	16.768	3.304	-96.250	-73.628	32.183
600	17.590	26.543	18.140	5.042	-95.985	-69.130	25.180
700	17.930	29.281	19.541	6.818	-95.707	-64.675	20.192
800	18.220	31.695	20.913	8.626	-95.419	-60.261	16.462
900	18.470	33.855	22.232	10.461	-95.123	-55.885	13.571
1000	18.700	35.813	23.493	12.320	-94.821	-51.541	11.264
1100	18.910	37.605	24.696	14.200	-94.520	-47.228	9.383
1200*	19.120	39.260	25.842	16.102	-94.218	-42.941	7.820
1300	19.320	40.798	26.933	18.024	-93.920	-38.680	6.503
1400	19.520	42.237	27.976	19.966	-93.626	-34.441	5.376
1500	19.710	43.591	28.973	21.927	-93.338	-30.227	4.404
1600	19.900	44.869	29.927	23.908	-93.054	-26.027	3.555
1700	20.090	46.081	30.842	25.907	-92.781	-21.847	2.809
1800	20.270	47.234	31.720	27.925	-92.515	-17.680	2.147
1900	20.460	48.335	32.566	29.962	-92.262	-13.530	1.556
2000	20.640	49.389	33.381	32.017	-92.022	-9.392	1.026

*Data extrapolated above 1200 K.

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

298.15-2000 K: $C_p^\circ = 17.132 + 1.784 \times 10^{-3}T - 2.199 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 17.132 \times 10^{-3}T + 0.892 \times 10^{-6}T^2 + 2.199 \times 10^{-2}T^3 - 5.925$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -98.678 + 4.412 \times 10^{-3}T - 0.613 \times 10^{-6}T^2 + 210.800T^{-1}$
 $\Delta G_r^\circ = -98.678 - 4.412 \times 10^{-3}T \ln T + 0.613 \times 10^{-6}T^2 + 105.400T^{-1} + 76.771 \times 10^{-3}T$

Source: Data from Chase (17) who extrapolated data above 1200 K.

Mo₂S₃(c)
Dimolybdenum Trisulfide
[Formation: 2Mo(c) + 3S(c,l) = Mo₂S₃(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H _{2,98} °)/T	H°- H _{2,98} °	ΔHf°	ΔGf°	
298.15	26.122	27.480	27.480	0	-97.300	-94.556	69.311
300*	26.168	27.642	27.482	.048	-97.304	-94.540	68.871
368.3	27.470	33.161	28.036	1.888	-97.414	-93.899	55.719
368.3	27.470	33.161	28.036	1.888	-97.702	-93.899	55.719
388.36	27.852	34.628	28.339	2.443	-97.742	-93.689	52.723
388.36	27.852	34.628	28.339	2.443	-98.981	-93.689	52.723
400	28.074	35.454	28.534	2.768	-99.058	-93.530	51.102
432.02	28.492	37.632	29.129	3.674	-99.326	-93.079	47.086
500	29.380	41.865	30.577	5.644	-100.207	-92.016	40.220
600	30.449	47.319	32.924	8.637	-101.035	-90.296	32.890
700	31.407	52.085	35.328	11.730	-101.616	-88.455	27.617
717.824	31.567	52.877	35.754	12.291	-101.696	-88.118	26.828

*Data above 298 K estimated. Mo₂S₃ metastable below 900 K.

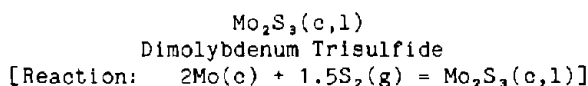
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2080 K: $C_p^\circ = 26.360 + 7.880 \times 10^{-3}T - 2.300 \times 10^{-5}T^2$
 $H^\circ - H_{2,98}^\circ = 26.360 \times 10^{-3}T + 3.940 \times 10^{-6}T^2 + 2.300 \times 10^{-2}T^{-1} - 8.981$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -95.438 - 6.4916 \times 10^{-3}T + 6.721 \times 10^{-6}T^2 - 118.400T^{-1}$
 $\Delta G_f^\circ = -95.438 + 6.4916 \times 10^{-3}T \ln T - 6.721 \times 10^{-6}T^2 - 59.200T^{-1} - 33.776 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = -98.784 - 0.127 \times 10^{-3}T + 1.483 \times 10^{-6}T^2 + 348.400T^{-1}$
 $\Delta G_f^\circ = -98.784 + 0.127 \times 10^{-3}T \ln T - 1.483 \times 10^{-6}T^2 + 174.200T^{-1} + 11.773 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = -147.259 + 134.093 \times 10^{-3}T - 128.363 \times 10^{-6}T^2 + 6055.000T^{-1}$
 $\Delta G_f^\circ = -147.259 - 134.093 \times 10^{-3}T \ln T + 128.363 \times 10^{-6}T^2 + 3027.500T^{-1} + 867.458 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = -175.695 + 122.375 \times 10^{-3}T - 68.927 \times 10^{-6}T^2 + 15734.500T^{-1}$
 $\Delta G_f^\circ = -175.695 - 122.375 \times 10^{-3}T \ln T + 68.927 \times 10^{-6}T^2 + 7867.250T^{-1} + 861.916 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHr°	ΔGr°	
298.15	26.122	27.480	27.480	0	-143.365	-123.097	90.231
300*	26.168	27.642	27.482	.048	-143.360	-122.971	89.583
400	28.074	35.454	28.534	2.768	-143.011	-116.227	63.503
500	29.380	41.865	30.577	5.644	-142.590	-109.576	47.895
600	30.449	47.319	32.924	8.637	-142.118	-103.018	37.524
700	31.407	52.085	35.328	11.730	-141.591	-96.541	30.141
800	32.305	56.338	37.693	14.916	-141.010	-90.144	24.626
900	33.168	60.193	39.982	18.190	-140.374	-83.825	20.355
1000	34.010	63.732	42.183	21.549	-139.685	-77.580	16.955
1100	34.838	67.012	44.293	24.991	-138.954	-71.404	14.186
1200	35.656	70.078	46.315	28.516	-138.178	-65.294	11.891
1300	36.468	72.964	48.254	32.123	-137.364	-59.254	9.961
1400	37.275	75.697	50.118	35.810	-136.514	-53.276	8.317
1500	38.078	78.296	51.911	39.577	-135.632	-47.365	6.901
1600	38.878	80.779	53.638	43.425	-134.712	-41.507	5.670
1700	39.676	83.160	55.305	47.353	-133.767	-35.711	4.591
1800	40.473	85.450	56.917	51.360	-132.792	-29.969	3.639
1900	41.268	87.660	58.477	55.447	-131.797	-24.286	2.794
2000	42.062	89.797	59.990	59.614	-130.782	-18.653	2.038
2080	42.697	91.459	61.169	63.004	-129.956	-14.185	1.490
2080	37.500	106.363	61.169	94.004	-98.956	-14.185	1.490
2100	37.500	106.721	61.600	94.754	-98.854	-13.369	1.391
2140	37.500	107.429	62.450	96.254	-98.659	-11.743	1.199

*Data above 298 K estimated. Mo_2S_3 metastable below 900 K.

Phase changes: 2080 K, melting point of Mo_2S_3 ; $\Delta\text{H}^\circ = 31.000\text{kcal/mol}$.
 2140 K, decomposition point of Mo_2S_3 .

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

298.15-2080 K: $\text{Cp}^\circ = 26.360 + 7.880 \times 10^{-3}\text{T} - 2.300 \times 10^{-5}\text{T}^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 26.360 \times 10^{-3}\text{T} + 3.940 \times 10^{-6}\text{T}^2 + 2.300 \times 10^{-2}\text{T}^{-1} - 8.981$
 2080-2140 K: $\text{Cp}^\circ = 37.500$
 $\text{H}^\circ - \text{H}_{298}^\circ = 37.500 \times 10^{-3}\text{T} + 16.004$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta\text{Hr}^\circ = -145.805 + 5.091 \times 10^{-3}\text{T} + 1.090 \times 10^{-5}\text{T}^2 + 245.950\text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -145.805 - 5.091 \times 10^{-3}\text{TlnT} - 1.090 \times 10^{-6}\text{T}^2 + 122.975\text{T}^{-1} + 104.113 \times 10^{-3}\text{T}$
 2000-2080 K: $\Delta\text{Hr}^\circ = -142.730 + 3.341 \times 10^{-3}\text{T} + 1.420 \times 10^{-6}\text{T}^2 - 1541.600\text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -142.730 - 3.341 \times 10^{-3}\text{TlnT} - 1.420 \times 10^{-6}\text{T}^2 - 770.800\text{T}^{-1} + 90.154 \times 10^{-3}\text{T}$
 2080-2140 K: $\Delta\text{Hr}^\circ = -117.745 + 14.481 \times 10^{-3}\text{T} - 2.520 \times 10^{-6}\text{T}^2 - 1771.600\text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -117.745 - 14.481 \times 10^{-3}\text{TlnT} + 2.520 \times 10^{-6}\text{T}^2 - 885.800\text{T}^{-1} + 155.084 \times 10^{-3}\text{T}$

Source: Data from Chase (17) who estimated all above 298 K.

NS(g)
Nitrogen Sulfide (ideal gas)
[Formation: $0.5\text{N}_2(\text{g}) + \text{S}(\text{c,l}) = \text{NS}(\text{g})$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	7.599	53.057	53.057	0	63.300	56.588	-41.480
300	7.600	53.104	53.057	.014	63.298	56.547	-41.194
368.3	7.697	54.669	53.215	.535	63.197	55.020	-32.648
368.3	7.697	54.669	53.215	.535	63.101	55.020	-32.648
388.36	7.725	55.078	53.301	.690	63.067	54.581	-30.715
388.36	7.725	55.078	53.301	.690	62.654	54.581	-30.715
400	7.742	55.306	53.356	.780	62.615	54.340	-29.690
432.02	7.809	55.905	53.523	1.029	62.489	53.682	-27.156
500	7.951	57.056	53.926	1.565	62.111	52.329	-22.872
600	8.146	58.523	54.573	2.370	61.703	50.412	-18.362
700	8.306	59.791	55.230	3.193	61.362	48.558	-15.160
717.824	8.329	60	55.345	3.341	61.308	48.233	-14.685

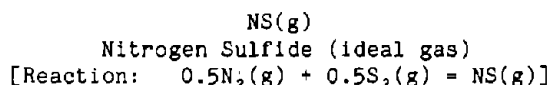
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-3000 K: $C_p^\circ = 8.067 + 0.470 \times 10^{-3}T - 0.541 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 8.067 \times 10^{-3}T + 0.235 \times 10^{-6}T^2 + 0.541 \times 10^{-2}T^{-1} - 2.608$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 64.483 - 3.365 \times 10^{-3}T + 1.658 \times 10^{-6}T^2 - 97.550T^{-1}$
 $\Delta G_f^\circ = 64.483 + 3.365 \times 10^{-3}T \ln T - 1.658 \times 10^{-6}T^2 - 48.775T^{-1} - 44.612 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = 63.368 - 1.102 \times 10^{-3}T - 0.089 \times 10^{-6}T^2 + 58.050T^{-1}$
 $\Delta G_f^\circ = 63.368 + 1.102 \times 10^{-3}T \ln T + 0.089 \times 10^{-6}T^2 + 29.025T^{-1} - 29.429 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = 47.210 + 43.638 \times 10^{-3}T - 43.371 \times 10^{-6}T^2 + 1960.250T^{-1}$
 $\Delta G_f^\circ = 47.210 - 43.638 \times 10^{-3}T \ln T + 43.371 \times 10^{-6}T^2 + 980.125T^{-1} + 255.799 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = 37.731 + 39.732 \times 10^{-3}T - 23.559 \times 10^{-6}T^2 + 5186.750T^{-1}$
 $\Delta G_f^\circ = 37.731 - 39.732 \times 10^{-3}T \ln T + 23.559 \times 10^{-6}T^2 + 2593.375T^{-1} + 253.952 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	7.599	53.057	53.057	0	47.945	47.075	-34.506
300	7.600	53.104	53.057	.014	47.945	47.069	-34.290
400	7.742	55.306	53.356	.780	47.964	46.774	-25.556
500	7.951	57.056	53.926	1.565	47.984	46.475	-20.314
600	8.146	58.523	54.573	2.370	48.008	46.171	-16.818
700	8.306	59.791	55.230	3.193	48.037	45.863	-14.319
800	8.433	60.909	55.872	4.030	48.068	45.550	-12.444
900	8.533	61.908	56.488	4.878	48.096	45.233	-10.984
1000	8.613	62.812	57.076	5.736	48.123	44.914	-9.816
1100	8.677	63.636	57.636	6.600	48.146	44.591	-8.859
1200	8.730	64.393	58.167	7.471	48.165	44.268	-8.062
1300	8.773	65.093	58.673	8.346	48.180	43.943	-7.387
1400	8.810	65.745	59.156	9.225	48.191	43.616	-6.809
1500	8.841	66.354	59.615	10.108	48.197	43.289	-6.307
1600	8.869	66.925	60.054	10.993	48.199	42.962	-5.868
1700	8.892	67.464	60.475	11.881	48.195	42.633	-5.481
1800	8.914	67.973	60.877	12.772	48.190	42.307	-5.137
1900	8.933	68.455	61.263	13.664	48.180	41.981	-4.829
2000	8.950	68.914	61.635	14.558	48.167	41.654	-4.552
2100	8.965	69.351	61.992	15.454	48.151	41.328	-4.301
2200	8.980	69.768	62.336	16.351	48.132	41.005	-4.073
2300	8.993	70.168	62.668	17.250	48.112	40.681	-3.866
2400	9.006	70.551	62.989	18.150	48.088	40.359	-3.675
2500	9.017	70.919	63.299	19.051	48.062	40.036	-3.500
2600	9.028	71.272	63.598	19.953	48.034	39.717	-3.338
2700	9.039	71.613	63.889	20.856	48.006	39.398	-3.189
2800	9.049	71.942	64.170	21.761	47.976	39.080	-3.050
2900	9.059	72.260	64.444	22.666	47.945	38.763	-2.921
3000	9.068	72.567	64.710	23.572	47.912	38.445	-2.801

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

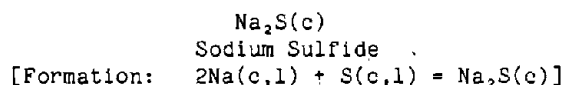
$$298.15\text{-}3000\text{ K: } \begin{aligned} \text{Cp}^\circ &= 8.067 + 0.470 \times 10^{-3}T - 0.541 \times 10^{-5}T^2 \\ \text{H}^\circ - \text{H}^\circ_{298} &= 8.067 \times 10^{-3}T + 0.235 \times 10^{-6}T^2 + 0.541 \times 10^{-2}T^{-1} - 2.608 \end{aligned}$$

Reaction equations (kcal/mol):

$$298.15\text{-}2000\text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= 47.694 + 0.637 \times 10^{-3}T - 0.220 \times 10^{-6}T^2 + 23.900T^{-1} \\ \Delta \text{Gr}^\circ &= 47.694 - 0.637 \times 10^{-3}T \ln T + 0.220 \times 10^{-6}T^2 + 11.950T^{-1} + 1.351 \times 10^{-3}T \end{aligned}$$

$$2000\text{-}3000\text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= 50.056 - 1.010 \times 10^{-3}T + 0.157 \times 10^{-6}T^2 - 1121.900T^{-1} \\ \Delta \text{Gr}^\circ &= 50.056 + 1.010 \times 10^{-3}T \ln T - 0.157 \times 10^{-6}T^2 - 560.950T^{-1} - 11.456 \times 10^{-3}T \end{aligned}$$

Sources: Enthalpy of formation at 298 K based on O'Hare (87), Gaydon (43), and Somayajulu (109).
Other data based on Herzberg (52).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	19.790	23.000	23.000	0	-87.500	-84.740	62.115
300	19.800	23.122	23.000	.037	-87.497	-84.721	61.718
368.3	20.039	27.208	23.415	1.397	-87.487	-84.094	49.901
368.3	20.039	27.208	23.415	1.397	-87.583	-84.094	49.901
371	20.049	27.354	23.443	1.451	-87.585	-84.069	49.523
371	20.049	27.354	23.443	1.451	-88.829	-84.069	49.523
388.36	20.109	28.273	23.638	1.800	-88.846	-83.845	47.183
388.36	20.109	28.273	23.638	1.800	-89.259	-83.845	47.183
400	20.150	28.867	23.782	2.034	-89.288	-83.682	45.721
432.02	20.262	30.423	24.217	2.681	-89.384	-83.231	42.104
500	20.500	33.402	25.268	4.067	-89.674	-82.235	35.945
600	20.850	37.171	26.946	6.135	-89.905	-80.723	29.403
700	21.200	40.411	28.642	8.238	-90.014	-79.184	24.722
717.824	21.262	40.945	28.941	8.616	-90.022	-78.908	24.024

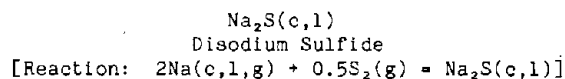
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1100 K: $C_p^\circ = 17.885 + 4.746 \times 10^{-3}T + 0.436 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 17.885 \times 10^{-3}T + 2.373 \times 10^{-6}T^2 - 0.436 \times 10^{-2}T^{-1} - 5.397$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -86.907 + 1.809 \times 10^{-3}T - 5.226 \times 10^{-6}T^2 - 199.200T^{-1}$
 $\Delta G_f^\circ = -86.907 - 1.809 \times 10^{-3}T \ln T + 5.226 \times 10^{-6}T^2 - 99.600T^{-1} + 17.136 \times 10^{-3}T$
 368.3-371 K: $\Delta H_f^\circ = -88.022 + 4.072 \times 10^{-3}T - 6.972 \times 10^{-6}T^2 - 43.600T^{-1}$
 $\Delta G_f^\circ = -88.022 - 4.072 \times 10^{-3}T \ln T + 6.972 \times 10^{-6}T^2 - 21.800T^{-1} + 32.319 \times 10^{-3}T$
 371-388.36 K: $\Delta H_f^\circ = -88.798 - 2.034 \times 10^{-3}T + 2.528 \times 10^{-6}T^2 + 138.200T^{-1}$
 $\Delta G_f^\circ = -88.798 + 2.034 \times 10^{-3}T \ln T - 2.528 \times 10^{-6}T^2 + 69.100T^{-1} + 1.151 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -104.956 + 42.706 \times 10^{-3}T - 40.754 \times 10^{-6}T^2 + 2040.400T^{-1}$
 $\Delta G_f^\circ = -104.956 - 42.706 \times 10^{-3}T \ln T + 40.754 \times 10^{-6}T^2 + 1020.200T^{-1} + 286.380 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -114.435 + 38.800 \times 10^{-3}T - 20.942 \times 10^{-6}T^2 + 5266.900T^{-1}$
 $\Delta G_f^\circ = -114.435 - 38.800 \times 10^{-3}T \ln T + 20.942 \times 10^{-6}T^2 + 2633.450T^{-1} + 284.532 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	19.790	23.000	23.000	0	-102.855	-94.254	69.089
300	19.800	23.122	23.000	.037	-102.849	-94.198	68.623
371	20.049	27.354	23.443	1.451	-102.723	-92.170	54.295
371	20.049	27.354	23.443	1.451	-103.967	-92.170	54.295
400	20.150	28.867	23.782	2.034	-103.939	-91.248	49.855
500	20.500	33.402	25.268	4.067	-103.801	-88.089	38.503
600	20.850	37.171	26.946	6.135	-103.599	-84.964	30.948
700	21.200	40.411	28.642	8.238	-103.339	-81.879	25.564
800	21.550	43.266	30.297	10.375	-103.028	-78.834	21.536
900	21.830	45.821	31.881	12.546	-102.677	-75.830	18.414
1000	22.190	48.140	33.393	14.747	-102.299	-72.866	15.925
1100	26.400	50.388	34.835	17.108	-101.777	-69.949	13.897
1177	35.424	52.412	35.917	19.415	-100.897	-67.739	12.578
1177	35.424	52.412	35.917	19.415	-147.467	-67.739	12.578
1200	38.120	53.124	36.240	20.261	-146.958	-66.191	12.055
1276	50.650	55.840	37.306	23.650	-144.667	-61.113	10.467
1300	44.850	56.743	37.675	24.789	-143.876	-59.574	10.015
1400	32.780	59.544	39.143	28.562	-141.555	-53.183	8.302
1445	32.000	60.556	39.793	30.002	-140.770	-50.355	7.616
1445*	22.000	63.745	39.793	34.610	-136.162	-50.355	7.616
1500	22.000	64.567	40.687	35.820	-135.754	-47.100	6.862
1600	22.000	65.987	42.224	38.020	-135.013	-41.213	5.629
1700	22.000	67.321	43.662	40.220	-134.277	-35.375	4.548
1800	22.000	68.578	45.011	42.420	-133.543	-29.577	3.591
1900	22.000	69.768	46.284	44.620	-132.812	-23.821	2.740
2000	22.000	70.896	47.486	46.820	-132.085	-18.103	1.978

*Heat capacity of liquid estimated.

Phase changes: 371 K, melting point of Na; ΔH° = 0.622 kcal/mol.
1177 K, calculated boiling point of Na to ideal monatomic gas; ΔH° = 23.285 kcal/mol.
1276 K, second order transition point of Na₂S; ΔH° = 0 kcal/mol.
1445 K, melting point of Na₂S; ΔH° = 4.608 kcal/mol.

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

298.15-1100 K: Cp° = 17.885 + 4.746x10⁻³T + 0.436x10⁻⁵T²
H° - H₂₉₈° = 17.885x10⁻³T + 2.373x10⁻⁶T² - 0.436x10⁻⁹T³ - 5.397
1100-1276 K: Cp° = -139.167 + 148.434x10⁻³T
H° - H₂₉₈° = -139.167x10⁻³T + 74.217x10⁻⁶T² + 80.389
1276-1445 K: Cp° = 222.848 - 136.172x10⁻³T
H° - H₂₉₈° = 222.848x10⁻³T - 68.086x10⁻⁶T² - 149.848
1445-2000 K: Cp° = 22.000
H° - H₂₉₈° = 22.000x10⁻³T + 2.820

Reaction equations (kcal/mol):

298.15-371 K: ΔHr° = -103.696 + 5.811x10⁻³T - 7.103x10⁻⁶T² - 77.750T⁻¹
ΔGr° = -103.696 - 5.811x10⁻³TlnT + 7.103x10⁻⁶T² - 38.875T⁻¹ + 63.099x10⁻³T
371-1100 K: ΔHr° = -104.472 - 0.295x10⁻³T + 2.397x10⁻⁶T² + 104.050T⁻¹
ΔGr° = -104.472 + 0.295x10⁻³TlnT - 2.397x10⁻⁶T² + 52.025T⁻¹ + 31.931x10⁻³T
1100-1177 K: ΔHr° = -18.685 - 157.347x10⁻³T + 74.241x10⁻⁶T² + 147.650T⁻¹
ΔGr° = -18.685 + 157.347x10⁻³TlnT - 74.241x10⁻⁶T² + 73.825T⁻¹ - 1066.891x10⁻³T
1177-1276 K: ΔHr° = -69.611 - 153.273x10⁻³T + 74.049x10⁻⁶T² - 56.150T⁻¹
ΔGr° = -69.611 + 153.273x10⁻³TlnT - 74.049x10⁻⁶T² - 28.075T⁻¹ - 994.970x10⁻³T
1276-1445 K: ΔHr° = -299.848 + 208.743x10⁻³T - 68.254x10⁻⁶T² - 56.150T⁻¹
ΔGr° = -299.848 - 208.743x10⁻³TlnT + 68.254x10⁻⁶T² - 28.075T⁻¹ + 1592.833x10⁻³T
1445-2000 K: ΔHr° = -147.180 + 7.895x10⁻³T - 0.168x10⁻⁶T² - 56.150T⁻¹
ΔGr° = -147.180 - 7.895x10⁻³TlnT + 0.168x10⁻⁶T² - 28.075T⁻¹ + 124.221x10⁻³T

Source: Data from Chase (17) who estimated liquid heat capacity.

NbS(g)
Niobium Monosulfide (ideal gas)
[Formation: Nb(c) + S(c,l) = NbS(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15*	7.980	59.870	59.870	0	103.000	90.028	-65.991
300	7.990	59.920	59.870	.015	102.994	89.948	-65.527
368.3	8.250	61.594	60.042	.572	102.759	87.000	-51.625
368.3	8.250	61.594	60.042	.572	102.663	87.000	-51.625
388.36	8.326	62.033	60.134	.738	102.589	86.149	-48.480
388.36	8.326	62.033	60.134	.738	102.176	86.149	-48.480
400	8.370	62.280	60.192	.835	102.114	85.670	-46.807
432.02	8.428	62.927	60.371	1.104	101.924	84.360	-42.675
500	8.550	64.170	60.806	1.682	101.409	81.637	-35.683
600	8.650	65.730	61.493	2.542	100.789	77.750	-28.320
700	8.710	67.070	62.199	3.410	100.224	73.950	-23.088
717.824	8.717	67.289	62.322	3.565	100.128	73.283	-22.312

*Data estimated.

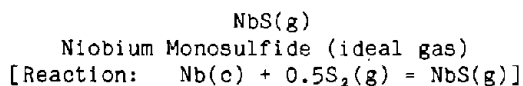
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 8.818 + 0.066x10⁻³T - 0.760x10⁻⁶T⁻²
H° - H₂₉₈° = 8.818x10⁻³T + 0.033x10⁻⁶T² + 0.760x10⁻²T⁻¹ - 2.887

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 104.468 - 4.552x10⁻³T + 0.978x10⁻⁶T² - 59.000T⁻¹
ΔGf° = 104.468 + 4.552x10⁻³T ln T - 0.978x10⁻⁶T² - 29.500T⁻¹ - 73.745x10⁻³T
368.3-388.36 K: ΔHf° = 103.353 - 2.289x10⁻³T - 0.768x10⁻⁶T² + 96.600T⁻¹
ΔGf° = 103.353 + 2.289x10⁻³T ln T + 0.768x10⁻⁶T² + 48.300T⁻¹ - 58.562x10⁻³T
388.36-432.02 K: ΔHf° = 87.195 + 42.451x10⁻³T - 44.050x10⁻⁶T² + 1998.800T⁻¹
ΔGf° = 87.195 - 42.451x10⁻³T ln T + 44.050x10⁻⁶T² + 999.400T⁻¹ + 226.666x10⁻³T
432.02-717.824 K: ΔHf° = 77.716 + 38.545x10⁻³T - 24.238x10⁻⁶T² + 5225.300T⁻¹
ΔGf° = 77.716 - 38.545x10⁻³T ln T + 24.238x10⁻⁶T² + 2612.650T⁻¹ + 224.819x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	7.980	59.870	59.870	0	87.645	80.514	-59.018
300	7.990	59.920	59.870	.015	87.642	80.471	-58.623
400	8.370	62.280	60.192	.835	87.463	78.104	-42.673
500	8.550	64.170	60.806	1.682	87.282	75.784	-33.125
600	8.650	65.730	61.493	2.542	87.094	73.509	-26.775
700	8.710	67.070	62.199	3.410	86.899	71.255	-22.247
800	8.750	68.240	62.885	4.284	86.693	69.032	-18.859
900	8.780	69.270	63.537	5.160	86.478	66.840	-16.231
1000	8.810	70.200	64.160	6.040	86.250	64.669	-14.133
1100	8.830	71.040	64.747	6.922	86.010	62.520	-12.421
1200	8.840	71.810	65.306	7.805	85.759	60.413	-11.002
1300	8.860	72.520	65.835	8.691	85.497	58.315	-9.804
1400	8.870	73.170	66.329	9.577	85.218	56.239	-8.779
1500	8.880	73.780	66.803	10.465	84.921	54.185	-7.895
1600	8.890	74.360	67.264	11.354	84.605	52.141	-7.122
1700	8.900	74.900	67.698	12.244	84.271	50.125	-6.444
1800	8.910	75.410	68.113	13.135	83.918	48.124	-5.843
1900	8.920	75.890	68.508	14.026	83.543	46.135	-5.307
2000	8.930	76.350	68.890	14.919	83.147	44.182	-4.828

*All data estimated

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

298.15-2000 K: $\text{Cp}^\circ = 8.818 + 0.066 \times 10^{-3}T - 0.760 \times 10^{-5}T^{-2}$
 $\text{H}^\circ - \text{H}_{298}^\circ = 8.818 \times 10^{-3}T + 0.033 \times 10^{-6}T^2 + 0.760 \times 10^{-2}T^{-1} - 2.887$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta \text{Hr}^\circ = 87.679 - 0.550 \times 10^{-3}T - 0.899 \times 10^{-6}T^2 + 62.450T^{-1}$
 $\Delta \text{Gr}^\circ = 87.679 + 0.550 \times 10^{-3}T \ln T + 0.899 \times 10^{-6}T^2 + 31.225T^{-1} - 27.782 \times 10^{-3}T$

Source: Data are those estimated by Mills (80).

NdS(c)
Neodymium Monosulfide
[Formation: Nd(c) + S(c,l) = NdS(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	11.930	20.650	20.650	0	-111.000	-109.774	80.466
300*	11.943	20.724	20.651	.022	-110.999	-109.766	79.963
368.3	12.261	23.213	20.902	.851	-111.010	-109.485	64.968
368.3	12.261	23.213	20.902	.851	-111.106	-109.485	64.968
388.36	12.355	23.865	21.038	1.098	-111.114	-109.396	61.562
388.36	12.355	23.865	21.038	1.098	-111.527	-109.396	61.562
400	12.409	24.231	21.126	1.242	-111.551	-109.332	59.735
432.02	12.492	25.190	21.392	1.641	-111.637	-109.151	55.217
500	12.667	27.030	22.036	2.497	-111.939	-108.735	47.528
600	12.845	29.356	23.068	3.773	-112.265	-108.061	39.361
700	12.983	31.347	24.111	5.065	-112.562	-107.334	33.511
717.824	13.004	31.674	24.295	5.297	-112.613	-107.199	32.638

*Data extrapolated above 298 K.

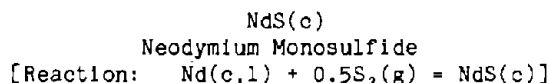
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 12.585 + 0.800x10⁻³T - 0.795x10⁻⁵T⁻²
H°- H₂₉₈° = 12.585x10⁻³T + 0.400x10⁻⁶T² + 0.795x10⁻²T⁻¹ - 4.054

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -111.044 + 0.443x10⁻³T - 0.848x10⁻⁶T² - 3.700T⁻¹
ΔGf° = -111.044 - 0.443x10⁻³TlnT + 0.848x10⁻⁶T² - 1.850T⁻¹ + 6.552x10⁻³T
368.3-388.36 K: ΔHf° = -112.159 + 2.706x10⁻³T - 2.594x10⁻⁶T² + 151.900T⁻¹
ΔGf° = -112.159 - 2.706x10⁻³TlnT + 2.594x10⁻⁶T² + 75.950T⁻¹ + 21.735x10⁻³T
388.36-432.02 K: ΔHf° = -128.318 + 47.446x10⁻³T - 45.876x10⁻⁶T² + 2054.100T⁻¹
ΔGf° = -128.318 - 47.446x10⁻³TlnT + 45.876x10⁻⁶T² + 1027.050T⁻¹ + 306.963x10⁻³T
432.02-717.824 K: ΔHf° = -137.796 + 43.540x10⁻³T - 26.064x10⁻⁶T² + 5280.600T⁻¹
ΔGf° = -137.796 - 43.540x10⁻³TlnT + 26.064x10⁻⁶T² + 2640.300T⁻¹ + 305.115x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	11.930	20.650	20.650	0	-126.355	-119.288	87.439
300*	11.943	20.724	20.651	.022	-126.351	-119.243	86.867
400	12.409	24.231	21.126	1.242	-126.202	-116.897	63.869
500	12.667	27.030	22.036	2.497	-126.066	-114.589	50.086
600	12.845	29.356	23.068	3.773	-125.959	-112.302	40.906
700	12.983	31.347	24.111	5.065	-125.887	-110.029	34.352
800	13.101	33.089	25.128	6.369	-125.860	-107.769	29.441
900	13.207	34.638	26.099	7.685	-125.887	-105.508	25.620
1000	13.306	36.035	27.025	9.010	-125.973	-103.239	22.563
1100	13.400	37.307	27.902	10.346	-126.125	-100.959	20.058
1128	13.425	37.644	28.139	10.722	-126.180	-100.323	19.437
1128	13.425	37.644	28.139	10.722	-126.904	-100.323	19.437
1200	13.490	38.477	28.735	11.690	-127.028	-98.624	17.962
1289	13.569	39.445	29.441	12.895	-127.176	-96.516	16.364
1289	13.569	39.445	29.441	12.895	-128.883	-96.516	16.364
1300	13.579	39.560	29.526	13.044	-128.900	-96.243	16.180
1400	13.665	40.570	30.280	14.406	-129.049	-93.725	14.631
1500	13.750	41.515	30.997	15.777	-129.191	-91.205	13.288
1600	13.835	42.406	31.683	17.156	-129.330	-88.668	12.111
1700	13.918	43.247	32.339	18.544	-129.464	-86.118	11.071
1800	14.001	44.045	32.967	19.940	-129.592	-83.566	10.146
1900	14.084	44.804	33.570	21.344	-129.715	-81.004	9.317
2000	14.166	45.528	34.150	22.756	-129.834	-78.436	8.571

*Data extrapolated 300-1300 K.

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: $\text{Cp}^\circ = 12.585 + 0.800 \times 10^{-3}T - 0.795 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 12.585 \times 10^{-3}T + 0.400 \times 10^{-6}T^2 + 0.795 \times 10^{-2}T^{-1} - 4.054$

Reaction equations (kcal/mol):

298.15-1128 K: $\Delta\text{Hr}^\circ = -127.833 + 4.445 \times 10^{-3}T - 2.725 \times 10^{-6}T^2 + 117.750T^{-1}$
 $\Delta\text{Gr}^\circ = -127.833 - 4.445 \times 10^{-3}T \ln T + 2.725 \times 10^{-6}T^2 + 58.875T^{-1} + 52.515 \times 10^{-3}T$
1128-1289 K: $\Delta\text{Hr}^\circ = -124.719 - 2.244 \times 10^{-3}T + 0.240 \times 10^{-6}T^2 + 45.350T^{-1}$
 $\Delta\text{Gr}^\circ = -124.719 + 2.244 \times 10^{-3}T \ln T - 0.240 \times 10^{-6}T^2 + 22.675T^{-1} + 6.108 \times 10^{-3}T$
1289-2000 K: $\Delta\text{Hr}^\circ = -126.604 - 2.106 \times 10^{-3}T + 0.240 \times 10^{-6}T^2 + 45.350T^{-1}$
 $\Delta\text{Gr}^\circ = -126.604 + 2.106 \times 10^{-3}T \ln T - 0.240 \times 10^{-6}T^2 + 22.675T^{-1} + 8.559 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Semakovich (105). Low-temperature heat capacities and entropy at 298 K from Vasilev (123). High-temperature data based on Fesenko (38). Data extrapolated from 300 to 1300 K.

NdS(g)
Neodymium Monosulfide (ideal gas)
[Formation: Nd(c) + S(c,l) = NdS(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	8.200	63.240	63.240	0	32.800	21.327	-15.633
300	8.210	63.290	63.240	.015	32.794	21.257	-15.486
368.3	8.415	65.001	63.411	.586	32.525	18.659	-11.072
368.3	8.415	65.001	63.411	.586	32.429	18.659	-11.072
388.36	8.475	65.449	63.505	.755	32.343	17.912	-10.080
388.36	8.475	65.449	63.505	.755	31.930	17.912	-10.080
400	8.510	65.700	63.565	.854	31.861	17.493	-9.557
432.02	8.555	66.357	63.748	1.127	31.649	16.350	-8.271
500	8.650	67.620	64.194	1.713	31.077	13.985	-6.113
600	8.730	69.200	64.897	2.582	30.344	10.641	-3.876
700	8.780	70.550	65.611	3.457	29.630	7.416	-2.315
717.824	8.785	70.771	65.737	3.614	29.504	6.853	-2.086

*Data except enthalpy of formation at 298 K estimated.

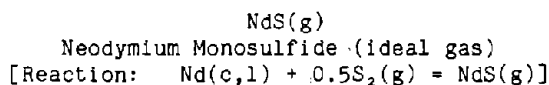
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 8.884 + 0.028x10⁻³T - 0.615x10⁻⁵T⁻²
H° - H°₂₉₈ = 8.884x10⁻³T + 0.014x10⁻⁵T² + 0.615x10⁻²T⁻¹ - 2.856

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 33.954 - 3.258x10⁻³T - 1.234x10⁻⁶T² - 21.700T⁻¹
ΔGf° = 33.954 + 3.258x10⁻³TlnT + 1.234x10⁻⁶T² - 10.850T⁻¹ - 61.158x10⁻³T
368.3-388.36 K: ΔHf° = 32.839 - 0.995x10⁻³T - 2.980x10⁻⁶T² + 133.900T⁻¹
ΔGf° = 32.839 + 0.995x10⁻³TlnT + 2.980x10⁻⁶T² + 66.950T⁻¹ - 45.975x10⁻³T
388.36-432.02 K: ΔHf° = 16.680 + 43.745x10⁻³T - 46.262x10⁻⁶T² + 2036.100T⁻¹
ΔGf° = 16.680 - 43.745x10⁻³TlnT + 46.262x10⁻⁶T² + 1018.050T⁻¹ + 239.254x10⁻³T
432.02-717.824 K: ΔHf° = 7.202 + 39.839x10⁻³T - 26.450x10⁻⁶T² + 5262.600T⁻¹
ΔGf° = 7.202 - 39.839x10⁻³TlnT + 26.450x10⁻⁶T² + 2631.300T⁻¹ + 237.406x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15*	8.200	63.240	63.240	0	17.445	11.814	-8.660
300	8.210	63.290	63.240	.015	17.442	11.780	-8.582
400	8.510	65.700	63.565	.854	17.210	9.927	-5.424
500	8.650	67.620	64.194	1.713	16.950	8.132	-3.555
600	8.730	69.200	64.897	2.582	16.649	6.400	-2.331
700	8.780	70.550	65.611	3.457	16.305	4.721	-1.474
800	8.810	71.730	66.309	4.337	15.908	3.086	-.843
900	8.830	72.770	66.971	5.219	15.448	1.507	-.366
1000	8.850	73.700	67.597	6.103	14.920	0.011	.003
1100	8.860	74.540	68.187	6.988	14.317	-1.473	.293
1128	8.866	74.763	68.348	7.236	14.135	-1.878	.364
1128	8.866	74.763	68.348	7.236	13.411	-1.878	.364
1200	8.880	75.310	68.747	7.875	12.956	-2.838	.517
1289	8.889	75.944	69.222	8.665	12.394	-3.994	.677
1289	8.889	75.944	69.222	8.665	10.687	-3.994	.677
1300	8.890	76.020	69.279	8.763	10.619	-4.122	.693
1400	8.890	76.680	69.786	9.652	9.997	-5.233	.817
1500	8.900	77.300	70.272	10.542	9.373	-6.317	.920
1600	8.910	77.870	70.724	11.433	8.747	-7.333	1.002
1700	8.910	78.410	71.161	12.324	8.117	-8.315	1.069
1800	8.920	78.920	71.578	13.215	7.483	-9.266	1.125
1900	8.930	79.400	71.975	14.108	6.849	-10.172	1.170
2000	8.930	79.860	72.359	15.001	6.211	-11.054	1.208

*Data except enthalpy of formation at 298 K estimated.

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: $C_p^\circ = 8.884 + 0.028 \times 10^{-3}T - 0.615 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 8.884 \times 10^{-3}T + 0.014 \times 10^{-6}T^2 + 0.615 \times 10^{-3}T^{-1} - 2.856$

Reaction equations (kcal/mol):

298.15-1128 K: $\Delta H_r^\circ = 17.165 + 0.744 \times 10^{-3}T - 3.111 \times 10^{-6}T^2 + 99.750T^{-1}$
 $\Delta G_r^\circ = 17.165 - 0.744 \times 10^{-3}T \ln T + 3.111 \times 10^{-6}T^2 + 49.875T^{-1} - 15.195 \times 10^{-3}T$
1128-1289 K: $\Delta H_r^\circ = 20.279 - 5.945 \times 10^{-3}T - 0.146 \times 10^{-6}T^2 + 27.350T^{-1}$
 $\Delta G_r^\circ = 20.279 + 5.945 \times 10^{-3}T \ln T + 0.146 \times 10^{-6}T^2 + 13.675T^{-1} - 61.601 \times 10^{-3}T$
1289-2000 K: $\Delta H_r^\circ = 18.394 - 5.808 \times 10^{-3}T - 0.146 \times 10^{-6}T^2 + 27.350T^{-1}$
 $\Delta G_r^\circ = 18.394 + 5.808 \times 10^{-3}T \ln T + 0.146 \times 10^{-6}T^2 + 13.675T^{-1} - 59.150 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schumm (104). Other data are those estimated by Mills (80).

Nd₂S₃(c)
Dineodymium Trisulfide
[Formation: 2Nd(c) + 3S(c,l) = Nd₂S₃(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	29.280	44.280	44.280	0	-269.000	-265.153	194.360
300*	29.310	44.460	44.280	.054	-268.998	-265.127	193.142
368.3	30.171	50.582	44.899	2.093	-269.022	-264.246	156.802
368.3	30.171	50.582	44.899	2.093	-269.310	-264.246	156.802
388.36	30.423	52.189	45.234	2.701	-269.332	-263.967	148.546
388.36	30.423	52.189	45.234	2.701	-270.571	-263.967	148.546
400	30.570	53.090	45.450	3.056	-270.640	-263.769	144.115
432.02	30.794	55.453	46.105	4.038	-270.891	-263.211	133.151
500	31.270	59.990	47.690	6.150	-271.769	-261.929	114.487
600	31.760	65.740	50.235	9.303	-272.677	-259.869	94.656
700	32.150	70.660	52.804	12.499	-273.459	-257.661	80.444
717.824	32.209	71.469	53.258	13.072	-273.589	-257.256	78.324

*Data above 298 K estimated.

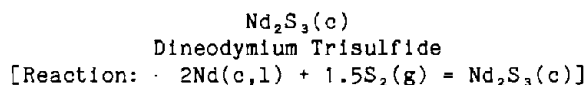
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 30.919 + 2.360x10⁻³T - 2.075x10⁻⁵T²
H°- H₂₉₈° = 30.919x10⁻³T + 1.180x10⁻⁶T² + 2.075x10⁻²T³ - 10.019

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -268.193 - 1.539x10⁻³T + 0.401x10⁻⁶T² - 114.500T⁻¹
ΔGf° = -268.193 + 1.539x10⁻³TlnT - 0.401x10⁻⁶T² - 57.250T⁻¹ + 2.190x10⁻³T
368.3-388.36 K: ΔHf° = -271.538 + 5.250x10⁻³T - 4.837x10⁻⁶T² + 352.300T⁻¹
ΔGf° = -271.538 - 5.250x10⁻³TlnT + 4.837x10⁻⁶T² + 176.150T⁻¹ + 47.739x10⁻³T
388.36-432.02 K: ΔHf° = -320.013 + 139.470x10⁻³T - 134.683x10⁻⁶T² + 6058.900T⁻¹
ΔGf° = -320.013 - 139.470x10⁻³TlnT + 134.683x10⁻⁶T² + 3029.450T⁻¹ + 903.424x10⁻³T
432.02-717.824 K: ΔHf° = -348.449 + 127.752x10⁻³T - 75.247x10⁻⁶T² + 15738.400T⁻¹
ΔGf° = -348.449 - 127.752x10⁻³TlnT + 75.247x10⁻⁶T² + 7869.200T⁻¹ + 897.882x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H _{2,98} °)/T	H°- H _{2,98} °	ΔHr°	ΔGr°	
298.15	29.280	44.280	44.280	0	-315.065	-293.694	215.281
300*	29.310	44.460	44.280	.054	-315.054	-293.558	213.854
400	30.570	53.090	45.450	3.056	-314.593	-286.466	156.516
500	31.270	59.990	47.690	6.150	-314.152	-279.488	122.163
600	31.760	65.740	50.235	9.303	-313.760	-272.592	99.290
700	32.150	70.660	52.804	12.499	-313.434	-265.747	82.969
800	32.480	74.980	55.316	15.731	-313.193	-258.960	70.744
900	32.790	78.820	57.716	18.994	-313.053	-252.193	61.240
1000	33.070	82.290	60.002	22.288	-313.026	-245.431	53.638
1100	33.340	85.460	62.180	25.608	-313.129	-238.675	47.420
1128	33.416	86.299	62.768	26.543	-313.182	-236.790	45.877
1128	33.416	86.299	62.768	26.543	-314.630	-236.790	45.877
1200	33.610	88.370	64.240	28.956	-314.728	-231.817	42.219
1289	33.833	90.782	65.990	31.958	-314.835	-225.674	38.263
1289	33.833	90.782	65.990	31.958	-318.249	-225.674	38.263
1300	33.860	91.070	66.201	32.330	-318.259	-224.889	37.807
1400	34.120	93.590	68.069	35.729	-318.340	-217.703	33.985
1500	34.370	95.950	69.848	39.153	-318.406	-210.528	30.673
1600	34.610	98.180	71.554	42.602	-318.457	-203.337	27.774
1700	34.860	100.280	73.176	46.076	-318.496	-196.124	25.213
1800	35.100	102.280	74.739	49.574	-318.518	-188.929	22.939
1900	35.350	104.180	76.235	53.096	-318.526	-181.717	20.902
2000	35.590	106.000	77.678	56.643	-318.518	-174.516	19.070

*Data above 298 K estimated.

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: $C_p^\circ = 30.919 + 2.360 \times 10^{-3}T - 2.075 \times 10^{-5}T^2$
 $H^\circ - H_{2,98}^\circ = 30.919 \times 10^{-3}T + 1.180 \times 10^{-6}T^2 + 2.075 \times 10^{-2}T^3 - 10.019$

Reaction equations (kcal/mol):

298.15-1128 K: $\Delta H_r^\circ = -318.559 + 10.469 \times 10^{-3}T - 5.230 \times 10^{-6}T^2 + 249.850T^{-1}$
 $\Delta G_r^\circ = -318.559 - 10.469 \times 10^{-3}T \ln T + 5.230 \times 10^{-6}T^2 + 124.925T^{-1} + 140.080 \times 10^{-3}T$
1128-1289 K: $\Delta H_r^\circ = -312.332 - 2.912 \times 10^{-3}T + 0.700 \times 10^{-6}T^2 + 105.050T^{-1}$
 $\Delta G_r^\circ = -312.332 + 2.912 \times 10^{-3}T \ln T - 0.700 \times 10^{-6}T^2 + 52.525T^{-1} + 47.267 \times 10^{-3}T$
1289-2000 K: $\Delta H_r^\circ = -316.101 - 2.636 \times 10^{-3}T + 0.700 \times 10^{-6}T^2 + 105.050T^{-1}$
 $\Delta G_r^\circ = -316.101 + 2.636 \times 10^{-3}T \ln T - 0.700 \times 10^{-6}T^2 + 52.525T^{-1} + 52.168 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Semakovich (105). Low-temperature heat capacities and entropy at 298 K from Nogteva (86). Data above 298 K estimated.

NiS(c)
Nickel Monosulfide
[Formation: $\text{Ni(c)} + \text{S(c,l)} = \text{NiS(c)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	11.260	12.660	12.660	0	-22.100	-21.462	15.732
300	11.294	12.730	12.660	.021	-22.101	-21.457	15.632
368.3	11.875	15.109	12.898	.814	-22.131	-21.309	12.645
368.3	11.875	15.109	12.898	.814	-22.227	-21.309	12.645
388.36	12.045	15.744	13.029	1.054	-22.240	-21.258	11.963
388.36	12.045	15.744	13.029	1.054	-22.653	-21.258	11.963
400	12.144	16.101	13.113	1.195	-22.679	-21.216	11.592
432.02	12.364	17.045	13.370	1.587	-22.771	-21.096	10.672
500	12.832	18.887	13.999	2.444	-23.077	-20.807	9.095
600	13.454	21.282	15.017	3.759	-23.401	-20.323	7.403
623	13.592	21.790	15.257	4.070	-23.472	-20.201	7.087
623*	13.640	24.037	15.257	5.470	-22.072	-20.201	7.087
631	13.699	24.211	15.369	5.579	-22.102	-20.177	6.988
700	14.210	25.659	16.313	6.542	-22.216	-19.957	6.231
717.824	14.342	26.018	16.550	6.796	-22.230	-19.899	6.058

*a-NiS metastable below 623 K.

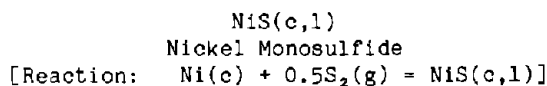
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 623 K, $\beta - \alpha$ transition point of NiS; $\Delta H^\circ = 1.400$ kcal/mol.
 631 K, Curie temperature of Ni; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-623 K: $C_p^\circ = 10.394 + 5.412 \times 10^{-3}T - 0.663 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 10.394 \times 10^{-3}T + 2.706 \times 10^{-6}T^2 + 0.663 \times 10^{-2}T^{-1} - 3.562$
 623-1250 K: $C_p^\circ = 9.052 + 7.378 \times 10^{-3}T - 0.035 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 9.052 \times 10^{-3}T + 3.689 \times 10^{-6}T^2 + 0.035 \times 10^{-2}T^{-1} - 1.607$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -21.780 - 0.776 \times 10^{-3}T + 0.143 \times 10^{-6}T^2 - 30.300T^{-1}$
 $\Delta G_f^\circ = -21.780 + 0.776 \times 10^{-3}T \ln T - 0.143 \times 10^{-6}T^2 - 15.150T^{-1} - 3.141 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -22.895 + 1.487 \times 10^{-3}T - 1.603 \times 10^{-6}T^2 + 125.300T^{-1}$
 $\Delta G_f^\circ = -22.895 - 1.487 \times 10^{-3}T \ln T + 1.603 \times 10^{-6}T^2 + 62.650T^{-1} + 12.041 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -39.053 + 46.227 \times 10^{-3}T - 44.885 \times 10^{-6}T^2 + 2027.500T^{-1}$
 $\Delta G_f^\circ = -39.053 - 46.227 \times 10^{-3}T \ln T + 44.885 \times 10^{-6}T^2 + 1013.750T^{-1} + 297.270 \times 10^{-3}T$
 432.02-623 K: $\Delta H_f^\circ = -48.532 + 42.321 \times 10^{-3}T - 25.073 \times 10^{-6}T^2 + 5254.000T^{-1}$
 $\Delta G_f^\circ = -48.532 - 42.321 \times 10^{-3}T \ln T + 25.073 \times 10^{-6}T^2 + 2627.000T^{-1} + 295.422 \times 10^{-3}T$
 623-631 K: $\Delta H_f^\circ = -46.576 + 40.979 \times 10^{-3}T - 24.090 \times 10^{-6}T^2 + 5191.200T^{-1}$
 $\Delta G_f^\circ = -46.576 - 40.979 \times 10^{-3}T \ln T + 24.090 \times 10^{-6}T^2 + 2595.600T^{-1} + 284.342 \times 10^{-3}T$
 631-717.824 K: $\Delta H_f^\circ = -44.028 + 32.655 \times 10^{-3}T - 17.065 \times 10^{-6}T^2 + 5132.200T^{-1}$
 $\Delta G_f^\circ = -44.028 - 32.655 \times 10^{-3}T \ln T + 17.065 \times 10^{-6}T^2 + 2566.100T^{-1} + 231.142 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	11.260	12.660	12.660	0	-37.455	-30.975	22.705
300	11.294	12.730	12.660	.021	-37.453	-30.935	22.536
400	12.144	16.101	13.113	1.195	-37.330	-28.781	15.725
500	12.832	18.887	13.999	2.444	-37.205	-26.660	11.653
600	13.454	21.282	15.017	3.759	-37.096	-24.564	8.947
623	13.592	21.790	15.257	4.070	-37.077	-24.082	8.448
623*	13.640	24.037	15.257	5.470	-35.677	-24.082	8.448
631	13.699	24.211	15.369	5.579	-35.677	-23.933	8.289
700	14.210	25.659	16.313	6.542	-35.541	-22.652	7.072
800	14.949	27.605	17.605	8.000	-35.256	-20.833	5.691
900	15.688	29.408	18.817	9.532	-34.912	-19.051	4.626
1000	16.426	31.099	19.961	11.138	-34.511	-17.312	3.783
1100	17.164	32.699	21.047	12.817	-34.057	-15.604	3.100
1200	17.902	34.225	22.083	14.570	-33.552	-13.953	2.541
1250	18.271	34.963	22.583	15.475	-33.278	-13.144	2.298
1250	17.000	40.563	22.583	22.475	-26.278	-13.144	2.298
1300	17.000	41.230	23.288	23.325	-26.066	-12.623	2.122
1400	17.000	42.489	24.614	25.025	-25.660	-11.601	1.811
1500	17.000	43.662	25.845	26.725	-25.278	-10.612	1.546
1600	17.000	44.759	26.993	28.425	-24.924	-9.642	1.317

*α-NiS metastable below 623 K. Data extrapolated 1066-1250 K. Enthalpy of fusion and heat capacity of liquid estimated.

Phase changes: 623 K, β - α transition point of NiS; ΔH° = 1.400 kcal/mol.

631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.

1250 K, liquidus temperature of NiS, with melting beginning at 1066 K. Data extrapolated to give total enthalpy of fusion isothermally at 1250 K.

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

298.15-623 K: Cp° = 10.394 + 5.412x10⁻³T - 0.663x10⁻⁵T²
H° - H°₂₉₈ = 10.394x10⁻³T + 2.706x10⁻⁶T² + 0.663x10⁻²T³ - 3.562
623-1250 K: Cp° = 9.052 + 7.378x10⁻³T - 0.035x10⁻⁵T²
H° - H°₂₉₈ = 9.052x10⁻³T + 3.689x10⁻⁶T² + 0.035x10⁻²T³ - 1.607
1250-1600 K: Cp° = 17.000
H° - H°₂₉₈ = 17.000x10⁻³T + 1.225

Reaction equations (kcal/mol):

298.15-623 K: ΔHr° = -38.569 + 3.227x10⁻³T - 1.734x10⁻⁶T² + 91.150T⁻¹
ΔGr° = -38.569 - 3.227x10⁻³TlnT + 1.734x10⁻⁶T² + 45.575T⁻¹ + 42.822x10⁻³T
623-631 K: ΔHr° = -36.613 + 1.885x10⁻³T - 0.751x10⁻⁶T² + 28.350T⁻¹
ΔGr° = -36.613 - 1.885x10⁻³TlnT + 0.751x10⁻⁶T² + 14.175T⁻¹ + 31.741x10⁻³T
631-750 K: ΔHr° = -34.064 + 6.439x10⁻³T + 6.274x10⁻⁶T² - 30.650T⁻¹
ΔGr° = -34.064 + 6.439x10⁻³TlnT - 6.274x10⁻⁶T² - 15.325T⁻¹ - 21.459x10⁻³T
750-1250 K: ΔHr° = -36.974 - 0.191x10⁻³T + 2.372x10⁻⁶T² + 282.950T⁻¹
ΔGr° = -36.974 + 0.191x10⁻³TlnT - 2.372x10⁻⁶T² + 141.475T⁻¹ + 20.585x10⁻³T
1250-1600 K: ΔHr° = -34.143 + 7.758x10⁻³T - 1.317x10⁻⁶T² + 279.450T⁻¹
ΔGr° = -34.143 - 7.758x10⁻³TlnT + 1.317x10⁻⁶T² + 139.725T⁻¹ + 70.386x10⁻³T

Sources: All data to 1066 K from Mah (74) except enthalpy of transition at 623 K which is from Dubuc (33). Data extrapolated 1066-1250 K. Liquidus temperature from Kullerud (70). Heat capacity of liquid estimated.

NiS(g)
Nickel Monosulfide (ideal gas)
[Formation: Ni(c) + S(c,l) = NiS(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	8.234	60.272	60.272	0	85.425	71.868	-52.680
300	8.244	60.322	60.272	.015	85.418	71.784	-52.294
368.3	8.588	62.050	60.445	.591	85.171	68.705	-40.769
368.3	8.588	62.050	60.445	.591	85.075	68.705	-40.769
388.36	8.688	62.509	60.540	.765	84.995	67.816	-38.163
388.36	8.688	62.509	60.540	.765	84.582	67.816	-38.163
400	8.747	62.766	60.601	.866	84.517	67.314	-36.778
432.02	8.877	63.445	60.787	1.148	84.315	65.944	-33.359
500	9.153	64.763	61.241	1.761	83.765	63.097	-27.579
600	9.464	66.461	61.973	2.693	83.058	59.029	-21.501
631	9.533	66.939	62.205	2.987	82.831	57.795	-20.017
700	9.685	67.937	62.721	3.651	82.418	55.082	-17.197
717.824	9.710	68.181	62.854	3.824	82.323	54.388	-16.559

*Data except enthalpy of formation at 298 K estimated.

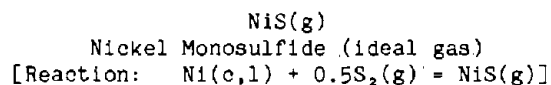
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2500 K: Cp° = 10.037 - 0.108x10⁻³T - 1.574x10⁻⁵T²
H° - H°₂₉₈ = 10.037x10⁻³T - 0.054x10⁻⁶T² + 1.574x10⁻²T³ - 3.516

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 85.792 - 1.133x10⁻³T - 2.617x10⁻⁶T² + 60.800T⁻¹
ΔGf° = 85.792 + 1.133x10⁻³TlnT + 2.617x10⁻⁶T² + 30.400T⁻¹ - 54.278x10⁻³T
368.3-388.36 K: ΔHf° = 84.676 + 1.130x10⁻³T - 4.363x10⁻⁶T² + 216.400T⁻¹
ΔGf° = 84.676 - 1.130x10⁻³TlnT + 4.363x10⁻⁶T² + 108.200T⁻¹ - 39.095x10⁻³T
388.36-432.02 K: ΔHf° = 68.518 + 45.870x10⁻³T - 47.645x10⁻⁶T² + 2118.600T⁻¹
ΔGf° = 68.518 - 45.870x10⁻³TlnT + 47.645x10⁻⁶T² + 1059.300T⁻¹ + 246.133x10⁻³T
432.02-631 K: ΔHf° = 59.039 + 41.964x10⁻³T - 27.833x10⁻⁶T² + 5345.100T⁻¹
ΔGf° = 59.039 - 41.964x10⁻³TlnT + 27.833x10⁻⁶T² + 2672.550T⁻¹ + 244.286x10⁻³T
631-717.824 K: ΔHf° = 61.588 + 33.640x10⁻³T - 20.808x10⁻⁶T² + 5286.100T⁻¹
ΔGf° = 61.588 - 33.640x10⁻³TlnT + 20.808x10⁻⁶T² + 2643.050T⁻¹ + 191.086x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	8.234	60.272	60.272	0	70.070	62.354	-45.706
300	8.244	60.322	60.272	.015	70.066	62.307	-45.390
400	8.747	62.766	60.601	.866	69.866	59.749	-32.645
500	9.153	64.763	61.241	1.761	69.638	57.244	-25.021
600	9.464	66.461	61.973	2.693	69.364	54.788	-19.956
631	9.533	66.939	62.205	2.987	69.256	54.039	-18.716
700	9.685	67.937	62.721	3.651	69.093	52.387	-16.356
800	9.827	69.240	63.456	4.627	68.896	50.011	-13.662
900	9.910	70.403	64.164	5.615	68.697	47.662	-11.574
1000	9.948	71.450	64.842	6.608	68.484	45.333	-9.907
1100	9.956	72.398	65.486	7.603	68.254	43.038	-8.551
1200	9.945	73.264	66.098	8.599	68.003	40.755	-7.422
1300	9.920	74.059	66.681	9.592	67.726	38.492	-6.471
1400	9.889	74.793	67.234	10.582	67.423	36.256	-5.660
1500	9.855	75.475	67.762	11.570	67.092	34.038	-4.959
1600	9.820	76.109	68.263	12.553	66.729	31.851	-4.351
1700	9.786	76.704	68.743	13.534	66.339	29.670	-3.814
1728	9.777	76.864	68.873	13.808	66.223	29.082	-3.678
1728	9.777	76.864	68.873	13.808	62.123	29.082	-3.678
1800	9.753	77.262	69.200	14.511	61.817	27.711	-3.365
1900	9.723	77.789	69.640	15.484	61.384	25.821	-2.970
2000	9.695	78.287	70.060	16.455	60.947	23.966	-2.619

*Data except 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.

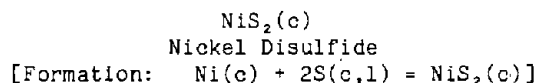
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $\text{Cp}^\circ = 10.037 - 0.108 \times 10^{-3}T - 1.574 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 10.037 \times 10^{-3}T - 0.054 \times 10^{-6}T^2 + 1.574 \times 10^{-2}T^{-1} - 3.516$

Reaction equations (kcal/mol):

298.15-631 K: $\Delta\text{Hr}^\circ = 69.003 + 2.869 \times 10^{-3}T - 4.494 \times 10^{-6}T^2 + 182.250T^{-1}$
 $\Delta\text{Gr}^\circ = 69.003 - 2.869 \times 10^{-3}T \ln T + 4.494 \times 10^{-6}T^2 + 91.125T^{-1} - 8.315 \times 10^{-3}T$
631-750 K: $\Delta\text{Hr}^\circ = 71.552 - 5.455 \times 10^{-3}T + 2.531 \times 10^{-6}T^2 + 123.250T^{-1}$
 $\Delta\text{Gr}^\circ = 71.552 + 5.455 \times 10^{-3}T \ln T - 2.531 \times 10^{-6}T^2 + 61.625T^{-1} - 61.515 \times 10^{-3}T$
750-1728 K: $\Delta\text{Hr}^\circ = 68.642 + 0.794 \times 10^{-3}T - 1.371 \times 10^{-6}T^2 + 436.850T^{-1}$
 $\Delta\text{Gr}^\circ = 68.642 - 0.794 \times 10^{-3}T \ln T + 1.371 \times 10^{-6}T^2 + 218.425T^{-1} - 19.471 \times 10^{-3}T$
1728-2000 K: $\Delta\text{Hr}^\circ = 68.576 - 3.435 \times 10^{-3}T - 0.214 \times 10^{-6}T^2 + 123.250T^{-1}$
 $\Delta\text{Gr}^\circ = 68.576 + 3.435 \times 10^{-3}T \ln T + 0.214 \times 10^{-6}T^2 + 61.625T^{-1} - 48.908 \times 10^{-3}T$

Source: Data from Chase (17) who estimated all except enthalpy of formation at 298 K.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15*	16.880	17.200	17.200	0	-31.400	-29.831	21.867
300	16.889	17.304	17.201	.031	-31.401	-29.821	21.724
368.3	17.228	20.802	17.554	1.196	-31.443	-29.459	17.481
368.3	17.228	20.802	17.554	1.196	-31.635	-29.459	17.481
388.36	17.327	21.718	17.745	1.543	-31.660	-29.339	16.510
388.36	17.327	21.718	17.745	1.543	-32.486	-29.339	16.510
400	17.385	22.231	17.869	1.745	-32.539	-29.244	15.978
432.02	17.544	23.576	18.242	2.304	-32.727	-28.974	14.657
500	17.881	26.164	19.148	3.508	-33.360	-28.330	12.383
600	18.377	29.468	20.600	5.321	-34.043	-27.259	9.929
631	18.531	30.398	21.058	5.893	-34.244	-26.902	9.318
700	18.873	32.338	22.075	7.184	-34.578	-26.077	8.142
717.824	18.961	32.814	22.336	7.521	-34.646	-25.859	7.873

*Data except enthalpy of formation at 298 K estimated.

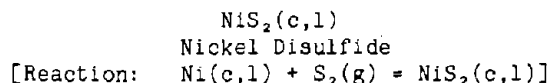
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1280 K: Cp° = 15.402 + 4.958x10⁻³T
 H° - H₂₉₈° = 15.402x10⁻³T + 2.479x10⁻⁶T² - 4.812

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -29.524 - 3.942x10⁻³T + 1.633x10⁻⁶T² - 252.200T⁻¹
 ΔGf° = -29.524 + 3.942x10⁻³TlnT - 1.633x10⁻⁶T² - 126.100T⁻¹ - 21.585x10⁻³T
 368.3-388.36 K: ΔHf° = -31.754 + 0.584x10⁻³T - 1.859x10⁻⁶T² + 59.000T⁻¹
 ΔGf° = -31.754 - 0.584x10⁻³TlnT + 1.859x10⁻⁶T² + 29.500T⁻¹ + 8.781x10⁻³T
 388.36-432.02 K: ΔHf° = -64.071 + 90.064x10⁻³T - 88.423x10⁻⁶T² + 3863.400T⁻¹
 ΔGf° = -64.071 - 90.064x10⁻³TlnT + 88.423x10⁻⁶T² + 1931.700T⁻¹ + 579.238x10⁻³T
 432.02-631 K: ΔHf° = -83.028 + 82.252x10⁻³T - 48.799x10⁻⁶T² + 10316.400T⁻¹
 ΔGf° = -83.028 - 82.252x10⁻³TlnT + 48.799x10⁻⁶T² + 5158.200T⁻¹ + 575.543x10⁻³T
 631-717.824 K: ΔHf° = -80.479 + 73.928x10⁻³T - 41.774x10⁻⁶T² + 10257.400T⁻¹
 ΔGf° = -80.479 - 73.928x10⁻³TlnT + 41.774x10⁻⁶T² + 5128.700T⁻¹ + 522.343x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	16.880	17.200	17.200	0	-62.110	-48.858	35.814
300	16.889	17.304	17.201	.031	-62.105	-48.776	35.533
400	17.385	22.231	17.869	1.745	-61.841	-44.375	24.245
500	17.881	26.164	19.148	3.508	-61.615	-40.037	17.500
600	18.377	29.468	20.600	5.321	-61.432	-35.741	13.019
631	18.531	30.398	21.058	5.893	-61.395	-34.413	11.919
700	18.873	32.338	22.075	7.184	-61.228	-31.467	9.824
800	19.369	34.890	23.520	9.096	-60.924	-27.238	7.441
900	19.865	37.200	24.914	11.057	-60.591	-23.050	5.597
1000	20.361	39.319	26.250	13.069	-60.228	-18.900	4.131
1100	20.857	41.283	27.528	15.130	-59.840	-14.776	2.936
1200	21.353	43.119	28.752	17.240	-59.428	-10.701	1.949
1280	21.750	44.510	29.694	18.964	-59.081	-7.468	1.275
1280	21.750	56.810	29.694	34.708	-43.337	-7.468	1.275
1300	21.750	57.147	30.114	35.143	-43.249	-6.908	1.161
1400	21.750	58.759	32.103	37.318	-42.826	-4.126	.644
1500	21.750	60.259	33.930	39.493	-42.432	-1.377	.201
1600	21.750	61.663	35.620	41.668	-42.068	1.351	-.185
1700	21.750	62.982	37.192	43.843	-41.734	4.042	-.520
1728	21.750	63.337	37.613	44.452	-41.646	4.810	-.608
1728	21.750	63.337	37.613	44.452	-45.746	4.810	-.608
1800	21.750	64.225	38.659	46.018	-45.530	6.911	-.839

*Data except enthalpy of formation at 298 K and temperature of fusion estimated.

Phase changes: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
1280 K, melting point of NiS₂; ΔH° = 15.744 kcal/mol.
1728 K, melting point of Ni; ΔH° = 4.100 kcal/mol.

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

298.15-1280 K: Cp° = 15.402 + 4.958x10⁻³T
H° - H₂₉₈° = 15.402x10⁻³T + 2.479x10⁻⁶T² - 4.812
1280-1800 K: Cp° = 21.750
H° - H₂₉₈° = 21.750x10⁻³T + 6.868

Reaction equations (kcal/mol):

298.15-631 K: ΔHr° = -63.102 + 4.063x10⁻³T - 2.121x10⁻⁶T² - 9.300T⁻¹
ΔGr° = -63.102 - 4.063x10⁻³TlnT + 2.121x10⁻⁶T² - 4.650T⁻¹ + 70.341x10⁻³T
631-750 K: ΔHr° = -60.553 - 4.261x10⁻³T + 4.904x10⁻⁶T² - 68.300T⁻¹
ΔGr° = -60.553 + 4.261x10⁻³TlnT - 4.904x10⁻⁶T² - 34.150T⁻¹ + 17.141x10⁻³T
750-1280 K: ΔHr° = -63.463 + 1.988x10⁻³T + 1.002x10⁻⁶T² + 245.300T⁻¹
ΔGr° = -63.463 - 1.988x10⁻³TlnT - 1.002x10⁻⁶T² + 122.650T⁻¹ + 59.185x10⁻³T
1280-1728 K: ΔHr° = -51.783 + 8.336x10⁻³T - 1.477x10⁻⁶T² + 245.300T⁻¹
ΔGr° = -51.783 - 8.336x10⁻³TlnT + 1.477x10⁻⁶T² + 122.650T⁻¹ + 92.304x10⁻³T
1728-1800 K: ΔHr° = -51.848 + 4.107x10⁻³T - 0.320x10⁻⁶T² - 68.300T⁻¹
ΔGr° = -51.848 - 4.107x10⁻³TlnT + 0.320x10⁻⁶T² - 34.150T⁻¹ + 62.868x10⁻³T

Source: Data from Chase (17) who estimated all except enthalpy of formation at 298 K and temperature of fusion.

Ni₃S₂(c)
Trinickel Disulfide
[Formation: 3Ni(c) + 2S(c,l) = Ni₃S₂(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	28.120	32.000	32.000	0	-52.100	-50.686	37.153
300	28.170	32.170	32.003	.050	-52.106	-50.678	36.918
368.3	29.714	38.127	32.597	2.037	-52.205	-50.344	29.874
368.3	29.714	38.127	32.597	2.037	-52.397	-50.344	29.874
388.36	30.167	39.715	32.924	2.637	-52.436	-50.230	28.267
388.36	30.167	39.715	32.924	2.637	-53.262	-50.230	28.267
400	30.430	40.610	33.135	2.990	-53.322	-50.139	27.394
432.02	30.917	42.972	33.778	3.972	-53.529	-49.877	25.232
500	31.950	47.570	35.350	6.110	-54.206	-49.249	21.526
600	33.350	53.520	37.887	9.380	-54.996	-48.184	17.551
631	33.902	55.214	38.697	10.422	-55.265	-47.819	16.562
700	35.130	58.790	40.504	12.800	-55.570	-46.980	14.668
717.824	35.570	59.679	40.969	13.430	-55.608	-46.759	14.236

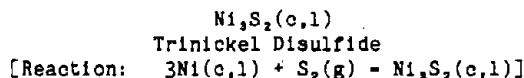
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-834 K: Cp° = 24.645 + 15.630x10⁻³T - 1.053x10⁻⁵T²
 H° - H₂₉₈° = 24.645x10⁻³T + 7.815x10⁻⁶T² + 1.053x10⁻²T⁻¹ - 8.396

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -51.656 - 0.691x10⁻³T - 1.591x10⁻⁶T² - 28.900T⁻¹
 ΔGf° = -51.656 + 0.691x10⁻³T lnT + 1.591x10⁻⁶T² - 14.450T⁻¹ - 0.997x10⁻³T
 368.3-388.36 K: ΔHf° = -53.886 + 3.835x10⁻³T - 5.083x10⁻⁶T² + 282.300T⁻¹
 ΔGf° = -53.886 - 3.835x10⁻³T lnT + 5.083x10⁻⁶T² + 141.150T⁻¹ + 29.369x10⁻³T
 388.36-432.02 K: ΔHf° = -86.202 + 93.315x10⁻³T - 91.647x10⁻⁶T² + 4086.700T⁻¹
 ΔGf° = -86.202 - 93.315x10⁻³T lnT + 91.647x10⁻⁶T² + 2043.350T⁻¹ + 599.825x10⁻³T
 432.02-631 K: ΔHf° = -105.160 + 85.503x10⁻³T - 52.023x10⁻⁶T² + 10539.700T⁻¹
 ΔGf° = -105.160 - 85.503x10⁻³T lnT + 52.023x10⁻⁶T² + 5269.850T⁻¹ + 596.130x10⁻³T
 631-717.824 K: ΔHf° = -97.513 + 60.531x10⁻³T - 30.948x10⁻⁶T² + 10362.700T⁻¹
 ΔGf° = -97.513 - 60.531x10⁻³T lnT + 30.948x10⁻⁶T² + 5181.350T⁻¹ + 436.531x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H _{2,98} °)/T	H° - H _{2,98} °	ΔHr°	ΔGr°	
298.15	28.120	32.000	32.000	0	-82.810	-69.713	51.101
300	28.170	32.170	32.003	.050	-82.810	-69.632	50.727
400	30.430	40.610	33.135	2.990	-82.624	-65.270	35.661
500	31.950	47.570	35.350	6.110	-82.461	-60.955	26.643
600	33.350	53.520	37.887	9.380	-82.385	-56.665	20.640
631	33.902	55.214	38.697	10.422	-82.415	-55.330	19.164
700	35.130	58.790	40.504	12.800	-82.220	-52.370	16.350
800	37.600	63.630	43.093	16.430	-81.672	-48.146	13.153
834	38.620	65.220	43.972	17.720	-81.438	-46.735	12.247
834	46.020	81.190	43.972	31.040	-68.118	-46.735	12.247
900	45.550	84.670	46.826	34.060	-67.166	-45.078	10.946
1000	44.840	89.440	50.860	38.580	-65.819	-42.712	9.335
1064	44.390	92.200	53.263	41.430	-65.028	-41.230	8.469
1064	45.200	96.620	53.263	46.130	-60.328	-41.230	8.469
1100	45.200	98.120	54.702	47.760	-59.868	-40.585	8.063
1200	45.200	102.050	58.483	52.280	-58.638	-38.892	7.083
1300	45.200	105.670	61.978	56.800	-57.472	-37.306	6.272
1400	45.200	109.020	65.220	61.320	-56.374	-35.791	5.587
1500	45.200	112.140	68.247	65.840	-55.349	-34.366	5.007
1600	45.200	115.060	71.085	70.360	-54.400	-32.992	4.506
1700	45.200	117.800	73.753	74.880	-53.525	-31.716	4.077
1728	45.200	118.538	74.473	76.146	-53.294	-31.313	3.960
1728	45.200	118.538	74.473	76.146	-65.594	-31.313	3.960
1800	45.200	120.380	76.269	79.400	-65.030	-29.896	3.630

Phase changes: 631 K, Curie temperature of Ni; ΔH° = 0 kcal/mol.
 834 K, α - β transition point of Ni₃S₂; ΔH° = 13.320 kcal/mol.
 1064 K, incongruent melting point of Ni₃S₂; ΔH° = 4.700 kcal/mol.
 1728 K, melting point of Ni; ΔH° = 4.100 kcal/mol.

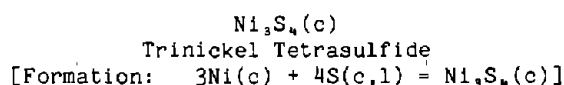
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-834 K: Cp° = 24.645 + 15.630x10⁻³T - 1.053x10⁻⁵T²
 H° - H_{2,98}° = 24.645x10⁻³T + 7.815x10⁻⁶T² + 1.053x10⁻⁵T³ - 8.396
 834-1064 K: Cp° = 47.696 - 4.092x10⁻³T + 12.082x10⁻⁵T²
 H° - H_{2,98}° = 47.696x10⁻³T - 2.046x10⁻⁶T² - 12.082x10⁻⁵T³ - 5.867
 1064-1800 K: Cp° = 45.200
 H° - H_{2,98}° = 45.200x10⁻³T - 1.963

Reaction equations (kcal/mol):

298.15-631 K: ΔHr° = -85.233 + 7.314x10⁻³T - 5.345x10⁻⁶T² + 214.000T⁻¹
 ΔGr° = -85.233 - 7.314x10⁻³TlnT + 5.345x10⁻⁶T² + 107.000T⁻¹ + 90.929x10⁻³T
 631-750 K: ΔHr° = -77.587 - 17.658x10⁻³T + 15.730x10⁻⁶T² + 37.000T⁻¹
 ΔGr° = -77.587 + 17.658x10⁻³TlnT - 15.730x10⁻⁶T² + 18.500T⁻¹ - 68.671x10⁻³T
 750-834 K: ΔHr° = -86.317 + 1.089x10⁻³T + 4.024x10⁻⁶T² + 977.800T⁻¹
 ΔGr° = -86.317 - 1.089x10⁻³TlnT - 4.024x10⁻⁶T² + 488.900T⁻¹ + 57.460x10⁻³T
 834-1064 K: ΔHr° = -83.787 + 24.140x10⁻³T - 5.837x10⁻⁶T² - 335.700T⁻¹
 ΔGr° = -83.787 - 24.140x10⁻³TlnT + 5.837x10⁻⁶T² - 167.850T⁻¹ + 202.194x10⁻³T
 1064-1728 K: ΔHr° = -79.883 + 21.644x10⁻³T - 3.791x10⁻⁶T² + 872.500T⁻¹
 ΔGr° = -79.883 - 21.644x10⁻³TlnT + 3.791x10⁻⁶T² + 436.250T⁻¹ + 182.771x10⁻³T
 1728-1800 K: ΔHr° = -80.080 + 8.957x10⁻³T - 0.320x10⁻⁶T² - 68.300T⁻¹
 ΔGr° = -80.080 - 8.957x10⁻³TlnT + 0.320x10⁻⁶T² - 34.150T⁻¹ + 94.462x10⁻³T

Sources: Data at 298 K from Mah (74). Other data from Ferrante (35).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15*	39.390	44.570	44.570	0	-71.968	-69.734	51.115
300	39.454	44.814	44.571	.073	-71.971	-69.719	50.790
368.3	41.799	53.138	45.406	2.848	-72.050	-69.202	41.064
368.3	41.799	53.138	45.406	2.848	-72.434	-69.202	41.064
388.36	42.487	55.373	45.864	3.693	-72.466	-69.022	38.842
388.36	42.487	55.373	45.864	3.693	-74.118	-69.022	38.842
400	42.887	56.634	46.159	4.190	-74.210	-68.869	37.628
432.02	43.987	59.979	47.061	5.581	-74.535	-68.432	34.618
500	46.321	66.573	49.273	8.650	-75.628	-67.376	29.449
600	49.754	75.322	52.899	13.454	-76.598	-65.632	23.906
631	50.819	77.855	54.063	15.013	-76.855	-65.054	22.531
700	53.188	83.249	56.676	18.601	-77.045	-63.742	19.901
717.824	53.800	84.594	57.353	19.554	-77.033	-63.401	19.303

*Data except enthalpy of formation at 298 K estimated.

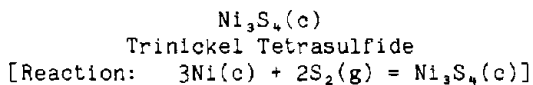
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 631 K, Curie temperature of Ni; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1100 K: $\text{Cp}^\circ = 29.148 + 34.344 \times 10^{-3}T$
 $\text{H}^\circ - \text{H}_{298}^\circ = 29.148 \times 10^{-3}T + 17.172 \times 10^{-6}T^2 - 10.217$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta \text{Hf}^\circ = -67.732 - 12.536 \times 10^{-3}T + 11.200 \times 10^{-6}T^2 - 445.400T^{-1}$
 $\Delta \text{Gf}^\circ = -67.732 + 12.536 \times 10^{-3}T \ln T - 11.200 \times 10^{-6}T^2 - 222.700T^{-1} - 72.294 \times 10^{-3}T$
 368.3-388.36 K: $\Delta \text{Hf}^\circ = -72.193 - 3.484 \times 10^{-3}T + 4.216 \times 10^{-6}T^2 + 177.000T^{-1}$
 $\Delta \text{Gf}^\circ = -72.193 + 3.484 \times 10^{-3}T \ln T - 4.216 \times 10^{-6}T^2 + 88.500T^{-1} - 11.562 \times 10^{-3}T$
 388.36-432.02 K: $\Delta \text{Hf}^\circ = -136.826 + 175.476 \times 10^{-3}T - 168.912 \times 10^{-6}T^2 + 7785.800T^{-1}$
 $\Delta \text{Gf}^\circ = -136.826 - 175.476 \times 10^{-3}T \ln T + 168.912 \times 10^{-6}T^2 + 3892.900T^{-1} + 1129.351 \times 10^{-3}T$
 432.02-631 K: $\Delta \text{Hf}^\circ = -174.741 + 159.852 \times 10^{-3}T - 89.664 \times 10^{-6}T^2 + 20691.800T^{-1}$
 $\Delta \text{Gf}^\circ = -174.741 - 159.852 \times 10^{-3}T \ln T + 89.664 \times 10^{-6}T^2 + 10345.900T^{-1} + 1121.962 \times 10^{-3}T$
 631-717.824 K: $\Delta \text{Hf}^\circ = -167.094 + 134.880 \times 10^{-3}T - 68.589 \times 10^{-6}T^2 + 20514.800T^{-1}$
 $\Delta \text{Gf}^\circ = -167.094 - 134.880 \times 10^{-3}T \ln T + 68.589 \times 10^{-6}T^2 + 10257.400T^{-1} + 962.362 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/T$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHr°	ΔGr°	
298.15*	39.390	44.570	44.570	0	-133.388	-107.788	79.010
300	39.454	44.814	44.571	.073	-133.379	-107.628	78.406
400	42.887	56.634	46.159	4.190	-132.814	-99.132	54.162
500	46.321	66.573	49.273	8.650	-132.138	-90.788	39.683
600	49.754	75.322	52.899	13.454	-131.376	-82.596	30.085
631	50.819	77.855	54.063	15.013	-131.156	-80.076	27.734
700	53.188	83.249	56.676	18.601	-130.345	-74.522	23.267
800	56.622	90.576	50.461	24.092	-128.807	-66.657	18.210
900	60.055	97.443	64.192	29.926	-126.977	-58.999	14.327
1000	63.489	103.948	67.845	36.103	-124.860	-51.564	11.269

*Data except enthalpy of formation at 298 K estimated.

Phase change: 631 K, Curie temperature of Ni; $\Delta\text{H}^\circ = 0$ kcal/mol.

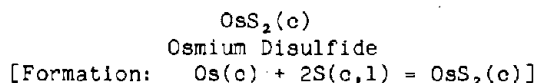
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $\text{Cp}^\circ = 29.148 + 34.344 \times 10^{-3}T$
 $\text{H}^\circ - \text{H}_{298}^\circ = 29.148 \times 10^{-3}T + 17.172 \times 10^{-6}T^2 - 10.217$

Reaction equations (kcal/mol):

298.15-631 K: $\Delta\text{Hr}^\circ = -134.887 + 3.474 \times 10^{-3}T + 3.692 \times 10^{-6}T^2 + 40.400T^{-1}$
 $\Delta\text{Gr}^\circ = -134.887 - 3.474 \times 10^{-3}T \ln T - 3.692 \times 10^{-6}T^2 + 20.200T^{-1} + 111.558 \times 10^{-3}T$
 631-750 K: $\Delta\text{Hr}^\circ = -127.241 - 21.498 \times 10^{-3}T + 24.767 \times 10^{-6}T^2 - 136.600T^{-1}$
 $\Delta\text{Gr}^\circ = -127.241 + 21.498 \times 10^{-3}T \ln T - 24.767 \times 10^{-6}T^2 - 68.300T^{-1} - 48.042 \times 10^{-3}T$
 750-1000 K: $\Delta\text{Hr}^\circ = -135.971 - 2.751 \times 10^{-3}T + 13.061 \times 10^{-6}T^2 + 804.200T^{-1}$
 $\Delta\text{Gr}^\circ = -135.971 + 2.751 \times 10^{-3}T \ln T - 13.061 \times 10^{-6}T^2 + 402.100T^{-1} + 78.089 \times 10^{-3}T$

Source: Data from Chase (17) who estimated all except enthalpy of formation at 298 K. Chase cites evidence that Ni_3S_4 decomposes near 630 K.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15*	14.860	13.000	13.000	0	-35.300	-32.282	23.663
300	14.900	13.090	13.000	.030	-35.301	-32.260	23.501
368.3	15.788	16.259	13.319	1.083	-35.421	-31.559	18.727
368.3	15.788	16.259	13.319	1.083	-35.613	-31.559	18.727
388.36	16.049	17.104	13.493	1.402	-35.652	-31.336	17.634
388.36	16.049	17.104	13.493	1.402	-36.478	-31.336	17.634
400	16.200	17.580	13.605	1.590	-36.536	-31.182	17.037
432.02	16.443	18.837	13.947	2.113	-36.732	-30.747	15.554
500	16.960	21.280	14.780	3.250	-37.354	-29.749	13.003
600	17.490	24.420	16.137	4.970	-37.962	-28.171	10.261
700	17.930	27.150	17.507	6.750	-38.405	-26.492	8.271
717.824	17.999	27.602	17.752	7.070	-38.471	-26.187	7.973

*Data except enthalpy of formation at 298 K estimated.

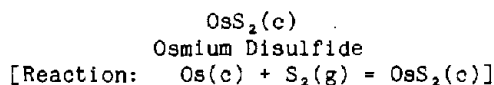
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1400 K: Cp° = 16.380 + 2.830x10⁻³T - 2.100x10⁻⁵T²
H°- H₂₉₈° = 16.380x10⁻³T + 1.415x10⁻⁶T² + 2.100x10⁻²T⁻¹ - 5.714

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -33.680 - 5.604x10⁻³T + 4.395x10⁻⁶T² - 101.200T⁻¹
ΔGf° = -33.680 + 5.604x10⁻³TlnT - 4.395x10⁻⁶T² - 50.600T⁻¹ - 25.360x10⁻³T
368.3-388.36 K: ΔHf° = -35.911 - 1.078x10⁻³T + 0.903x10⁻⁶T² + 210 T⁻¹
ΔGf° = -35.911 + 1.078x10⁻³TlnT - 0.903x10⁻⁶T² + 105.000T⁻¹ + 5.006x10⁻³T
388.36-432.02 K: ΔHf° = -68.227 + 88.402x10⁻³T - 85.661x10⁻⁶T² + 4014.400T⁻¹
ΔGf° = -68.227 - 88.402x10⁻³TlnT + 85.661x10⁻⁶T² + 2007.200T⁻¹ + 575.463x10⁻³T
432.02-717.824 K: ΔHf° = -87.185 + 80.590x10⁻³T - 46.037x10⁻⁶T² + 10467.400T⁻¹
ΔGf° = -87.185 - 80.590x10⁻³TlnT + 46.037x10⁻⁶T² + 5233.700T⁻¹ + 571.768x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	14.860	13.000	13.000	0	-66.010	-51.309	37.610
300	14.900	13.090	13.000	.030	-66.005	-51.214	37.309
400	16.200	17.580	13.605	1.590	-65.838	-46.313	25.304
500	16.960	21.280	14.780	3.250	-65.609	-41.455	18.120
600	17.490	24.420	16.137	4.970	-65.351	-36.652	13.350
700	17.930	27.150	17.507	6.750	-65.055	-31.882	9.954
800	18.320	29.570	18.870	8.560	-64.747	-27.168	7.422
900	18.670	31.750	20.183	10.410	-64.418	-22.492	5.462
1000	19.000	33.730	21.440	12.290	-64.075	-17.852	3.902
1100	19.320	35.560	22.642	14.210	-63.709	-13.248	2.632
1200	19.630	37.250	23.792	16.150	-63.338	-8.678	1.580
1300	19.930	38.840	24.894	18.130	-62.944	-4.146	.697
1400	20.230	40.320	25.934	20.140	-62.538	.375	-.059

*Data except enthalpy of formation at 298 K estimated.

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

298.15-1400 K: $C_p^\circ = 16.380 + 2.830 \times 10^{-3}T - 2.100 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 16.380 \times 10^{-3}T + 1.415 \times 10^{-6}T^2 + 2.100 \times 10^{-2}T^{-1} - 5.714$

Reaction equations (kcal/mol):

298.15-1400 K: $\Delta H_r^\circ = -67.258 + 2.401 \times 10^{-3}T + 0.641 \times 10^{-6}T^2 + 141.700T^{-1}$
 $\Delta G_r^\circ = -67.258 - 2.401 \times 10^{-3}T \ln T - 0.641 \times 10^{-6}T^2 + 70.850T^{-1} + 66.566 \times 10^{-3}T$

Source: Data from Mills (80) who estimated all except enthalpy of formation at 298 K.

PS(g)
Phosphorus Monosulfide (ideal gas)
[Formation: $P(c,1,1/4P_4(g)) + S(c,1) = PS(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	8.422	55.973	55.973	0	36.400	24.924	-18.269
300	8.426	56.025	55.973	.016	36.395	24.852	-18.105
317.3	8.457	56.498	55.988	.162	36.347	24.189	-16.661
317.3	8.457	56.498	55.988	.162	36.190	24.189	-16.661
368.3	8.547	57.768	56.149	.596	36.015	22.273	-13.217
368.3	8.547	57.768	56.149	.596	35.919	22.273	-13.217
388.36	8.582	58.222	56.245	.768	35.845	21.532	-12.117
388.36	8.582	58.222	56.245	.768	35.432	21.532	-12.117
400	8.603	58.476	56.306	.868	35.371	21.117	-11.537
432.02	8.639	59.140	56.492	1.144	35.183	19.982	-10.108
500	8.715	60.408	56.940	1.734	34.671	17.633	-7.707
550	8.752	61.241	57.295	2.171	34.356	15.930	-6.330
550	8.752	61.241	57.295	2.171	31.448	15.930	-6.330
600	8.788	62.004	57.656	2.609	31.233	14.530	-5.292
700	8.839	63.363	58.376	3.491	30.843	11.778	-3.677
717.824	8.846	63.585	58.502	3.649	30.779	11.294	-3.439

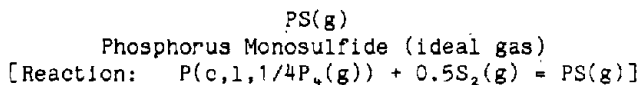
Phase changes: 317.3 K, melting point of P; $\Delta H^\circ = 0.157$ kcal/mol.
 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 550 K, boiling point of P; $\Delta H^\circ = 2.908$ kcal/mol of P.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-3000 K: $C_p^\circ = 8.843 + 0.108 \times 10^{-3}T - 0.403 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 8.843 \times 10^{-3}T + 0.054 \times 10^{-6}T^2 + 0.403 \times 10^2 T^{-1} - 2.777$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta H_f^\circ = 37.846 - 3.130 \times 10^{-3}T - 1.414 \times 10^{-6}T^2 - 115.300T^{-1}$
 $\Delta G_f^\circ = 37.846 + 3.130 \times 10^{-3}T \ln T + 1.414 \times 10^{-6}T^2 - 57.650T^{-1} - 60.947 \times 10^{-3}T$
 317.3-368.3 K: $\Delta H_f^\circ = 38.159 - 5.623 \times 10^{-3}T + 1.771 \times 10^{-6}T^2 - 115.300T^{-1}$
 $\Delta G_f^\circ = 38.159 + 5.623 \times 10^{-3}T \ln T - 1.771 \times 10^{-6}T^2 - 57.650T^{-1} - 75.283 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = 37.044 - 3.360 \times 10^{-3}T + 0.025 \times 10^{-6}T^2 + 40.300T^{-1}$
 $\Delta G_f^\circ = 37.044 + 3.360 \times 10^{-3}T \ln T - 0.025 \times 10^{-6}T^2 + 20.150T^{-1} - 60.101 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = 20.886 + 41.380 \times 10^{-3}T - 43.257 \times 10^{-6}T^2 + 1942.500T^{-1}$
 $\Delta G_f^\circ = 20.886 - 41.380 \times 10^{-3}T \ln T + 43.257 \times 10^{-6}T^2 + 971.250T^{-1} + 225.128 \times 10^{-3}T$
 432.02-550 K: $\Delta H_f^\circ = 11.407 + 37.474 \times 10^{-3}T - 23.445 \times 10^{-6}T^2 + 5169.000T^{-1}$
 $\Delta G_f^\circ = 11.407 - 37.474 \times 10^{-3}T \ln T + 23.445 \times 10^{-6}T^2 + 2584.500T^{-1} + 223.280 \times 10^{-3}T$
 550-717.824 K: $\Delta H_f^\circ = 7.947 + 38.812 \times 10^{-3}T - 23.449 \times 10^{-6}T^2 + 5068.700T^{-1}$
 $\Delta G_f^\circ = 7.947 - 38.812 \times 10^{-3}T \ln T + 23.449 \times 10^{-6}T^2 + 2534.350T^{-1} + 238.178 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H° ₂₉₈)/T	H°- H° ₂₉₈	ΔHr°	ΔGr°	
298.15	8.422	55.973	55.973	0	21.045	15.410	-11.296
300	8.426	56.025	55.973	.016	21.043	15.375	-11.201
317.3	8.457	56.498	55.988	.162	21.023	15.050	-10.366
317.3	8.457	56.498	55.988	.162	20.866	15.050	-10.366
400	8.603	58.476	56.306	.868	20.720	13.551	-7.404
500	8.715	60.408	56.940	1.734	20.544	11.780	-5.149
550	8.752	61.241	57.295	2.171	20.454	10.892	-4.328
550	8.752	61.241	57.295	2.171	17.546	10.892	-4.328
600	8.788	62.004	57.656	2.609	17.539	10.289	-3.748
700	8.839	63.363	58.376	3.491	17.518	9.083	-2.836
800	8.877	64.546	59.075	4.377	17.490	7.880	-2.153
900	8.905	65.593	59.742	5.266	17.458	6.680	-1.622
1000	8.928	66.533	60.375	6.158	17.421	5.485	-1.199
1100	8.947	67.384	60.973	7.052	17.381	4.294	-.853
1200	8.963	68.164	61.542	7.947	17.336	3.104	-.565
1300	8.977	68.882	62.079	8.844	17.288	1.919	-.323
1400	8.989	69.547	62.588	9.742	17.237	.740	-.116
1500	9.000	70.168	63.073	10.642	17.183	-.437	.064
1600	9.010	70.749	63.535	11.542	17.125	-1.609	.220
1700	9.020	71.296	63.976	12.444	17.065	-2.779	.357
1800	9.029	71.811	64.397	13.346	17.002	-3.942	.479
1900	9.038	72.300	64.800	14.250	16.936	-5.105	.587
2000	9.046	72.764	65.187	15.154	16.868	-6.263	.684

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
550 K, boiling point of P to P₄(g); ΔH° = 2.908 kcal/mol of P.

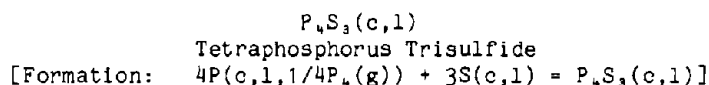
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $C_p^\circ = 8.843 + 0.108 \times 10^{-3}T - 0.403 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 8.843 \times 10^{-3}T + 0.054 \times 10^{-6}T^2 + 0.403 \times 10^{-2}T^{-1} - 2.777$

Reaction equations (kcal/mol):

298.15-317.3 K: $\Delta H_r^\circ = 21.057 + 0.873 \times 10^{-3}T - 3.291 \times 10^{-6}T^2 + 6.150T^{-1}$
 $\Delta G_r^\circ = 21.057 - 0.873 \times 10^{-3}T \ln T + 3.291 \times 10^{-6}T^2 + 3.075T^{-1} - 14.984 \times 10^{-3}T$
317.3-550 K: $\Delta H_r^\circ = 21.370 - 1.621 \times 10^{-3}T - 0.106 \times 10^{-6}T^2 + 6.150T^{-1}$
 $\Delta G_r^\circ = 21.370 + 1.621 \times 10^{-3}T \ln T + 0.106 \times 10^{-6}T^2 + 3.075T^{-1} - 29.320 \times 10^{-3}T$
550-2000 K: $\Delta H_r^\circ = 17.910 - 0.282 \times 10^{-3}T - 0.110 \times 10^{-6}T^2 - 94.150T^{-1}$
 $\Delta G_r^\circ = 17.910 + 0.282 \times 10^{-3}T \ln T + 0.110 \times 10^{-6}T^2 - 47.075T^{-1} - 14.423 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Drowart (32). Other data based on Dressler (31) and Narasimham (85).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	38.870	48.600	48.600	0	-41.100	-37.026	27.141
300	39.280	48.840	48.600	.072	-41.102	-37.003	26.956
313.9	40.500	50.610	48.665	.610	-41.109	-36.814	25.631
313.9	44.100	58.460	48.665	3.075	-38.644	-36.814	25.631
317.3	44.100	58.935	48.771	3.225	-38.630	-36.793	25.342
317.3	44.100	58.935	48.771	3.225	-39.258	-36.793	25.342
368.3	44.100	65.509	50.646	5.474	-39.158	-36.406	21.603
368.3	44.100	65.509	50.646	5.474	-39.446	-36.406	21.603
388.36	44.100	67.848	51.475	6.359	-39.423	-36.238	20.393
388.36	44.100	67.848	51.475	6.359	-40.662	-36.238	20.393
400	44.100	69.150	51.970	6.872	-40.706	-36.106	19.727
432.02	44.100	72.546	53.372	8.283	-40.889	-35.733	18.076
446	44.100	73.950	53.996	8.900	-41.148	-35.562	17.426
446	47.600	75.600	53.996	9.635	-40.413	-35.562	17.426
500	47.600	81.040	56.628	12.206	-40.699	-34.954	15.278
550	47.600	85.578	59.058	14.586	-40.887	-34.427	13.680
550	47.600	85.578	59.058	14.586	-52.519	-34.427	13.680
600	47.600	89.720	61.443	16.966	-52.334	-32.787	11.943
700	47.600	97.060	66.023	21.726	-51.862	-29.566	9.231

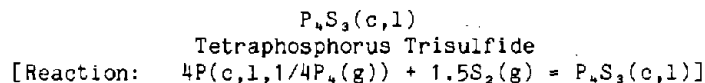
Phase changes: 313.9 K, α - β transition point of P_4S_3 ; $\Delta H^\circ = 2.465$ kcal/mol.
 317.3 K, melting point of P; $\Delta H^\circ = 0.157$ kcal/mol.
 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 446 K, melting point of P_4S_3 ; $\Delta H^\circ = 0.735$ kcal/mol.
 550 K, boiling point of P; $\Delta H^\circ = 2.908$ kcal/mol of P.

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

298.15-313.9 K: $C_p^\circ = 44.164 - 17.758 \times 10^{-3} T$
 $H^\circ - H^\circ_{298} = 44.164 \times 10^{-3} T - 8.879 \times 10^{-6} T^2 - 12.378$
 313.9-446 K: $C_p^\circ = 44.095$
 $H^\circ - H^\circ_{298} = 44.095 \times 10^{-3} T - 10.766$
 446-700 K: $C_p^\circ = 47.601$
 $H^\circ - H^\circ_{298} = 47.601 \times 10^{-3} T - 11.595$

Formation equations (kcal/mol):

298.15-313.9 K: $\Delta H_f^\circ = -39.396 + 4.446 \times 10^{-3} T - 16.468 \times 10^{-6} T^2 - 466.800 T^{-1}$
 $\Delta G_f^\circ = -39.396 - 4.446 \times 10^{-3} T \ln T + 16.468 \times 10^{-6} T^2 - 233.400 T^{-1} + 30.995 \times 10^{-3} T$
 313.9-317.3 K: $\Delta H_f^\circ = -37.784 + 4.377 \times 10^{-3} T - 7.589 \times 10^{-6} T^2 - 466.800 T^{-1}$
 $\Delta G_f^\circ = -37.784 - 4.377 \times 10^{-3} T \ln T + 7.589 \times 10^{-6} T^2 - 233.400 T^{-1} + 28.251 \times 10^{-3} T$
 317.3-368.3 K: $\Delta H_f^\circ = -36.531 + 5.595 \times 10^{-3} T + 5.151 \times 10^{-6} T^2 - 466.800 T^{-1}$
 $\Delta G_f^\circ = -36.531 + 5.595 \times 10^{-3} T \ln T - 5.151 \times 10^{-6} T^2 - 233.400 T^{-1} - 29.094 \times 10^{-3} T$
 368.3-388.36 K: $\Delta H_f^\circ = -39.876 + 1.194 \times 10^{-3} T - 0.087 \times 10^{-6} T^2$
 $\Delta G_f^\circ = -39.876 - 1.194 \times 10^{-3} T \ln T + 0.087 \times 10^{-6} T^2 + 16.454 \times 10^{-3} T$
 388.36-432.02 K: $\Delta H_f^\circ = -88.351 + 135.414 \times 10^{-3} T - 129.933 \times 10^{-6} T^2 + 5706.600 T^{-1}$
 $\Delta G_f^\circ = -88.351 - 135.414 \times 10^{-3} T \ln T + 129.933 \times 10^{-6} T^2 + 2853.300 T^{-1} + 872.140 \times 10^{-3} T$
 432.02-446 K: $\Delta H_f^\circ = -116.787 + 123.696 \times 10^{-3} T - 70.497 \times 10^{-6} T^2 + 15386.100 T^{-1}$
 $\Delta G_f^\circ = -116.787 - 123.696 \times 10^{-3} T \ln T + 70.497 \times 10^{-6} T^2 + 7693.050 T^{-1} + 866.597 \times 10^{-3} T$
 446-550 K: $\Delta H_f^\circ = -117.616 + 127.202 \times 10^{-3} T - 70.497 \times 10^{-6} T^2 + 15386.100 T^{-1}$
 $\Delta G_f^\circ = -117.616 - 127.202 \times 10^{-3} T \ln T + 70.497 \times 10^{-6} T^2 + 7693.050 T^{-1} + 889.843 \times 10^{-3} T$
 550-700 K: $\Delta H_f^\circ = -131.457 + 132.554 \times 10^{-3} T - 70.513 \times 10^{-6} T^2 + 14984.900 T^{-1}$
 $\Delta G_f^\circ = -131.457 - 132.554 \times 10^{-3} T \ln T + 70.513 \times 10^{-6} T^2 + 7492.450 T^{-1} + 949.434 \times 10^{-3} T$



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15	38.870	48.600	48.600	0	-87.165	-65.567	48.062
300	39.280	48.840	48.600	.072	-87.158	-65.434	47.668
313.9	40.500	50.610	48.665	.610	-87.100	-64.430	44.858
313.9	44.100	58.460	48.665	3.075	-84.635	-64.430	44.858
317.3	44.100	58.935	48.771	3.225	-84.604	-64.211	44.227
317.3	44.100	58.935	48.771	3.225	-85.232	-64.211	44.227
400	44.100	69.150	51.970	6.872	-84.659	-58.802	32.128
446	44.100	73.950	53.996	8.900	-84.355	-55.847	27.366
446	47.600	75.600	53.996	9.635	-83.620	-55.847	27.366
500	47.600	81.040	56.628	12.206	-83.081	-52.513	22.953
550	47.600	85.578	59.058	14.586	-82.595	-49.540	19.685
550	47.600	85.578	59.058	14.586	-94.227	-49.540	19.685
600	47.600	89.720	61.443	16.966	-93.418	-45.510	16.577
700	47.600	97.060	66.023	21.726	-91.837	-37.651	11.755

Phase changes: 313.9 K, $\alpha - \beta$ transition point of P_4S_3 ; $\Delta H^\circ = 2.465$ kcal/mol.
 317.3 K, melting point of P; $\Delta H^\circ = 0.157$ kcal/mol.
 446 K, melting point of P_4S_3 ; $\Delta H^\circ = 0.735$ kcal/mol.
 550 K, boiling point of P; $\Delta H^\circ = 2.908$ kcal/mol of P.

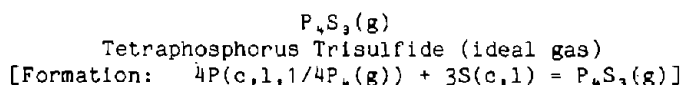
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-313.9 K: $C_p^\circ = 44.164 - 17.758 \times 10^{-3}T$
 $H^\circ - H_{298}^\circ = 44.164 \times 10^{-3}T - 8.879 \times 10^{-6}T^2 - 12.378$
 313.9-446 K: $C_p^\circ = 44.095$
 $H^\circ - H_{298}^\circ = 44.095 \times 10^{-3}T - 10.766$
 446-700 K: $C_p^\circ = 47.601$
 $H^\circ - H_{298}^\circ = 47.601 \times 10^{-3}T - 11.595$

Reaction equations (kcal/mol):

298.15-313.9 K: $\Delta H_r^\circ = -89.763 + 16.454 \times 10^{-3}T - 22.099 \times 10^{-6}T^2 - 102.450T^{-1}$
 $\Delta G_r^\circ = -89.763 - 16.454 \times 10^{-3}T \ln T + 22.099 \times 10^{-6}T^2 - 51.225T^{-1} + 168.884 \times 10^{-3}T$
 313.9-317.3 K: $\Delta H_r^\circ = -88.151 + 16.385 \times 10^{-3}T - 13.220 \times 10^{-6}T^2 - 102.450T^{-1}$
 $\Delta G_r^\circ = -88.151 - 16.385 \times 10^{-3}T \ln T + 13.220 \times 10^{-6}T^2 - 51.225T^{-1} + 166.140 \times 10^{-3}T$
 317.3-446 K: $\Delta H_r^\circ = -86.897 + 6.413 \times 10^{-3}T - 0.480 \times 10^{-6}T^2 - 102.450T^{-1}$
 $\Delta G_r^\circ = -86.897 - 6.413 \times 10^{-3}T \ln T + 0.480 \times 10^{-6}T^2 - 51.225T^{-1} + 108.795 \times 10^{-3}T$
 446-550 K: $\Delta H_r^\circ = -87.726 + 9.919 \times 10^{-3}T - 0.480 \times 10^{-6}T^2 - 102.450T^{-1}$
 $\Delta G_r^\circ = -87.726 - 9.919 \times 10^{-3}T \ln T + 0.480 \times 10^{-6}T^2 - 51.225T^{-1} + 132.040 \times 10^{-3}T$
 550-700 K: $\Delta H_r^\circ = -101.567 + 15.271 \times 10^{-3}T - 0.496 \times 10^{-6}T^2 - 503.650T^{-1}$
 $\Delta G_r^\circ = -101.567 - 15.271 \times 10^{-3}T \ln T + 0.496 \times 10^{-6}T^2 - 251.825T^{-1} + 191.631 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Cuelleron (28). Low-temperature heat capacities to 350 K and entropy at 298 K from Clever (21). High-temperature data based on Blachnik (10), Bouix (13), and Chattopadhyay (20).



T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	37.000	76.280	76.280	0	-35.850	-40.029	29.342
300	37.000	76.509	76.282	.068	-35.856	-40.057	29.181
317.3	37.000	78.583	76.352	.708	-35.896	-40.294	27.753
317.3	37.000	78.583	76.352	.708	-36.524	-40.294	27.753
368.3	37.000	84.098	77.052	2.595	-36.787	-40.880	24.258
368.3	37.000	84.098	77.052	2.595	-37.075	-40.880	24.258
388.36	37.000	86.060	77.467	3.337	-37.195	-41.082	23.119
388.36	37.000	86.060	77.467	3.337	-38.434	-41.082	23.119
400	37.000	87.153	77.733	3.768	-38.560	-41.161	22.489
432.02	37.000	90.002	78.538	4.953	-38.970	-41.355	20.920
500	37.000	95.409	80.473	7.468	-40.187	-41.626	18.194
550	37.000	98.936	81.994	9.318	-40.905	-41.791	16.606
550	37.000	98.936	81.994	9.318	-52.537	-41.791	16.606
600	37.000	102.155	83.542	11.168	-52.882	-40.796	14.860
700	37.000	107.859	86.619	14.868	-53.470	-38.733	12.093
717.824	37.000	108.789	87.158	15.527	-53.561	-38.355	11.678

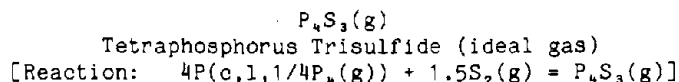
Phase changes: 317.3 K, melting point of P; $\Delta H^\circ = 0.157$ kcal/mol.
 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 550 K, boiling point of P; $\Delta H^\circ = 2.908$ kcal/mol of P.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2500 K: $C_p^\circ = 37.000$
 $H^\circ - H_{298}^\circ = 37.000 \times 10^{-3} T - 11.032$

Formation equations (kcal/mol):

298.15-317.3 K: $\Delta H_f^\circ = -32.799 - 2.718 \times 10^{-3} T - 7.589 \times 10^{-6} T^2 - 466.800 T^{-1}$
 $\Delta G_f^\circ = -32.799 + 2.718 \times 10^{-3} T \ln T + 7.589 \times 10^{-6} T^2 - 233.400 T^{-1} - 39.372 \times 10^{-3} T$
 317.3-368.3 K: $\Delta H_f^\circ = -31.546 - 12.690 \times 10^{-3} T + 5.151 \times 10^{-6} T^2 - 466.800 T^{-1}$
 $\Delta G_f^\circ = -31.546 + 12.690 \times 10^{-3} T \ln T - 5.151 \times 10^{-6} T^2 - 233.400 T^{-1} - 96.717 \times 10^{-3} T$
 368.3-388.36 K: $\Delta H_f^\circ = -34.891 - 5.901 \times 10^{-3} T - 0.087 \times 10^{-6} T^2$
 $\Delta G_f^\circ = -34.891 + 5.901 \times 10^{-3} T \ln T + 0.087 \times 10^{-6} T^2 - 51.168 \times 10^{-3} T$
 388.36-432.02 K: $\Delta H_f^\circ = -83.366 + 128.319 \times 10^{-3} T - 129.933 \times 10^{-6} T^2 + 5706.600 T^{-1}$
 $\Delta G_f^\circ = -83.366 - 128.319 \times 10^{-3} T \ln T + 129.933 \times 10^{-6} T^2 + 2853.300 T^{-1} + 804.517 \times 10^{-3} T$
 432.02-550 K: $\Delta H_f^\circ = -111.802 + 116.601 \times 10^{-3} T - 70.497 \times 10^{-6} T^2 + 15386.100 T^{-1}$
 $\Delta G_f^\circ = -111.802 - 116.601 \times 10^{-3} T \ln T + 70.497 \times 10^{-6} T^2 + 7693.050 T^{-1} + 798.974 \times 10^{-3} T$
 550-717.824 K: $\Delta H_f^\circ = -125.644 + 121.953 \times 10^{-3} T - 70.513 \times 10^{-6} T^2 + 14984.900 T^{-1}$
 $\Delta G_f^\circ = -125.644 - 121.953 \times 10^{-3} T \ln T + 70.513 \times 10^{-6} T^2 + 7492.450 T^{-1} + 858.565 \times 10^{-3} T$



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15	37.000	76.280	76.280	0	-81.915	-68.570	50.263
300	37.000	76.509	76.282	.068	-81.912	-68.489	49.894
317.3	37.000	78.583	76.352	.708	-81.870	-67.712	46.638
317.3	37.000	78.583	76.352	.708	-82.498	-67.712	46.638
400	37.000	87.153	77.733	3.768	-82.513	-63.858	34.890
500	37.000	95.409	80.473	7.468	-82.569	-59.186	25.870
550	37.000	98.936	81.994	9.318	-82.613	-56.904	22.611
550	37.000	98.936	81.994	9.318	-94.245	-56.904	22.611
600	37.000	102.155	83.542	11.168	-93.965	-53.519	19.494
700	37.000	107.859	86.619	14.868	-93.445	-46.818	14.617
800	37.000	112.800	89.590	18.568	-92.964	-40.190	10.979
900	37.000	117.158	92.416	22.268	-92.511	-33.622	8.164
1000	37.000	121.056	95.088	25.968	-92.082	-27.100	5.923
1100	37.000	124.582	97.611	29.668	-91.673	-20.622	4.097
1200	37.000	127.802	99.995	33.368	-91.282	-14.183	2.583
1300	37.000	130.763	102.249	37.068	-90.905	-7.775	1.307
1400	37.000	133.505	104.385	40.768	-90.545	-1.393	.217
1500	37.000	136.058	106.413	44.468	-90.199	4.959	-.723
1600	37.000	138.446	108.341	48.168	-89.863	11.295	-1.543
1700	37.000	140.689	110.178	51.868	-89.544	17.608	-2.264
1800	37.000	142.804	111.933	55.568	-89.231	23.905	-2.902
1900	37.000	144.804	113.610	59.268	-88.934	30.182	-3.472
2000	37.000	146.702	115.218	62.968	-88.642	36.445	-3.982

Phase changes: 317.3 K, melting point of P; $\Delta H^\circ = 0.157$ kcal/mol.

550 K, boiling point of P to $P_4(g)$; $\Delta H^\circ = 2.908$ kcal/mol of P.

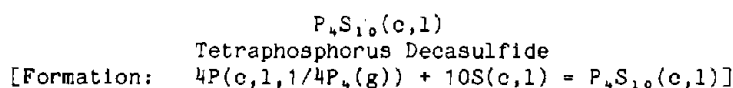
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2500 K: $C_p^\circ = 37.000$
 $H^\circ - H_{298}^\circ = 37.000 \times 10^{-3} T - 11.032$

Reaction equations (kcal/mol):

298.15-317.3 K: $\Delta H_r^\circ = -83.166 + 9.289 \times 10^{-3} T - 13.220 \times 10^{-6} T^2 - 102.450 T^{-1}$
 $\Delta G_r^\circ = -83.166 - 9.289 \times 10^{-3} T \ln T + 13.220 \times 10^{-6} T^2 - 51.225 T^{-1} + 98.517 \times 10^{-3} T$
 317.3-550 K: $\Delta H_r^\circ = -81.912 - 0.682 \times 10^{-3} T - 0.480 \times 10^{-6} T^2 - 102.450 T^{-1}$
 $\Delta G_r^\circ = -81.912 + 0.682 \times 10^{-3} T \ln T + 0.480 \times 10^{-6} T^2 - 51.225 T^{-1} + 41.172 \times 10^{-3} T$
 550-2000 K: $\Delta H_r^\circ = -95.754 + 4.669 \times 10^{-3} T - 0.496 \times 10^{-6} T^2 - 503.650 T^{-1}$
 $\Delta G_r^\circ = -95.754 - 4.669 \times 10^{-3} T \ln T + 0.496 \times 10^{-6} T^2 - 251.825 T^{-1} + 100.763 \times 10^{-3} T$

Source: Data from JANAF (30). Enthalpy of formation at 298 K based on P(white).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	70.740	91.240	91.240	0	-90.700	-83.351	61.097
300	70.877	91.678	91.241	.131	-90.713	-83.305	60.687
317.3	72.078	95.685	91.375	1.368	-90.821	-82.871	57.079
317.3	72.078	95.685	91.375	1.368	-91.449	-82.871	57.079
350	74.348	102.870	92.119	3.763	-91.716	-81.977	51.188
368.3	75.502	106.689	92.748	5.134	-91.856	-81.465	48.341
368.3	75.502	106.689	92.748	5.134	-92.816	-81.465	48.341
388.36	76.767	110.728	93.571	6.663	-92.982	-80.834	45.489
388.36	76.767	110.728	93.571	6.663	-97.112	-80.834	45.489
400	77.501	113.006	94.104	7.561	-97.387	-80.344	43.897
432.02	79.402	119.048	95.732	10.073	-98.311	-78.950	39.939
450	80.469	122.307	96.729	11.510	-99.548	-78.118	37.939
500	83.323	130.934	99.722	15.606	-101.228	-75.640	33.062
550	86.102	139.006	102.931	19.841	-102.613	-73.066	29.033
550	86.102	139.006	102.931	19.841	-114.245	-73.066	29.033
561	86.706	140.717	103.655	20.792	-114.443	-72.240	28.142
561	141.457	158.222	103.655	30.612	-104.623	-72.240	28.142
600	141.457	167.729	107.514	36.129	-103.099	-70.037	25.511
650	141.457	179.051	112.586	43.202	-101.017	-67.363	22.649
700	141.457	189.535	117.715	50.274	-98.842	-64.858	20.249
717.824	141.457	193.091	119.542	52.795	-98.031	-63.998	19.485

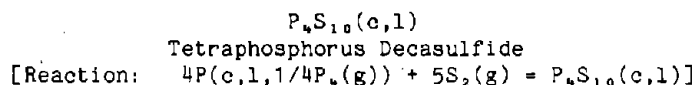
Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 550 K, boiling point of P; ΔH° = 2.908 kcal/mol of P.
 561 K, melting point of P₄S₁₀; ΔH° = 9.820 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-561 K: Cp° = 58.974 + 51.176x10⁻³T - 3.105x10⁻⁵T²
 H°- H₂₉₈° = 58.974x10⁻³T + 25.588x10⁻⁶T² + 3.105x10⁻²T³ - 20.899
 561-787 K: Cp° = 141.457
 H°- H₂₉₈° = 141.457x10⁻³T - 48.745

Formation equations (kcal/mol):

298.15-317.3 K: ΔHf° = -77.873 - 37.962x10⁻³T + 30.018x10⁻⁶T² - 1245.500T⁻¹
 ΔGf° = -77.873 + 37.962x10⁻³TlnT - 30.018x10⁻⁶T² - 622.750T⁻¹ - 218.710x10⁻³T
 317.3-368.3 K: ΔHf° = -76.619 - 47.934x10⁻³T + 42.758x10⁻⁶T² - 1245.500T⁻¹
 ΔGf° = -76.619 + 47.934x10⁻³TlnT - 42.758x10⁻⁶T² - 622.750T⁻¹ - 276.055x10⁻³T
 368.3-388.36 K: ΔHf° = -87.770 - 25.304x10⁻³T + 25.298x10⁻⁶T² + 310.500T⁻¹
 ΔGf° = -87.770 + 25.304x10⁻³TlnT - 25.298x10⁻⁶T² + 155.250T⁻¹ - 124.226x10⁻³T
 388.36-432.02 K: ΔHf° = -249.353 + 422.096x10⁻³T - 407.522x10⁻⁶T² + 19332.500T⁻¹
 ΔGf° = -249.353 - 422.096x10⁻³TlnT + 407.522x10⁻⁶T² + 9666.250T⁻¹ + 2728.058x10⁻³T
 432.02-550 K: ΔHf° = -344.140 + 383.036x10⁻³T - 209.402x10⁻⁶T² + 51597.500T⁻¹
 ΔGf° = -344.140 - 383.036x10⁻³TlnT + 209.402x10⁻⁶T² + 25798.750T⁻¹ + 2709.583x10⁻³T
 550-561 K: ΔHf° = -357.981 + 388.388x10⁻³T - 209.418x10⁻⁶T² + 51196.300T⁻¹
 ΔGf° = -357.981 - 388.388x10⁻³TlnT + 209.418x10⁻⁶T² + 25598.150T⁻¹ + 2769.174x10⁻³T
 561-717.824 K: ΔHf° = -385.828 + 470.871x10⁻³T - 235.006x10⁻⁶T² + 50885.800T⁻¹
 ΔGf° = -385.828 - 470.871x10⁻³TlnT + 235.006x10⁻⁶T² + 25442.900T⁻¹ + 3327.044x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H° ₂₉₈)/T	H°- H° ₂₉₈	ΔHr°	ΔGr°	
298.15	70.740	91.240	91.240	0	-244.250	-178.487	130.833
300	70.877	91.678	91.241	.131	-244.233	-178.078	129.728
317.3	72.078	95.685	91.375	1.368	-244.068	-174.264	120.028
317.3	72.078	95.685	91.375	1.368	-244.696	-174.264	120.028
350	74.348	102.870	92.119	3.763	-244.424	-167.025	104.294
400	77.501	113.006	94.104	7.561	-243.897	-156.000	85.233
450	80.469	122.307	96.729	11.510	-243.258	-145.046	70.443
500	83.323	130.934	99.722	15.606	-242.503	-134.172	58.646
550	86.102	139.006	102.931	19.841	-241.640	-123.441	49.050
550	86.102	139.006	102.931	19.841	-253.272	-123.441	49.050
561	86.706	140.717	103.655	20.792	-252.991	-120.847	47.078
561	141.457	158.222	103.655	30.612	-243.171	-120.847	47.078
600	141.457	167.729	107.514	36.129	-240.044	-112.446	40.958
650	141.457	179.051	112.586	43.202	-236.057	-101.973	34.286
700	141.457	189.535	117.715	50.274	-232.092	-91.809	28.664
750	141.457	199.294	122.831	57.347	-228.144	-81.923	23.872
787	141.457	206.106	126.588	62.581	-225.234	-74.780	20.766

Phase changes: 317.3 K, melting point of P; ΔH° = 0.157 kcal/mol.
 550 K, boiling point of P to P₄(g); ΔH° = 2.908 kcal/mol of P.
 561 K, melting point of P₄S₁₀; ΔH° = 9.820 kcal/mol.

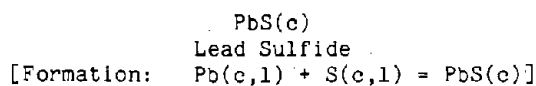
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-561 K: $C_p^\circ = 58.974 + 51.176 \times 10^{-3}T - 3.105 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 58.974 \times 10^{-3}T + 25.588 \times 10^{-6}T^2 + 3.105 \times 10^{-2}T^{-1} - 20.899$
 561-787 K: $C_p^\circ = 141.457$
 $H^\circ - H_{298}^\circ = 141.457 \times 10^{-3}T - 48.745$

Reaction equations (kcal/mol):

298.15-317.3 K: $\Delta H_r^\circ = -245.761 + 2.063 \times 10^{-3}T + 11.248 \times 10^{-6}T^2 - 31.000T^{-1}$
 $\Delta G_r^\circ = -245.761 - 2.063 \times 10^{-3}T \ln T - 11.248 \times 10^{-6}T^2 - 15.500T^{-1} + 240.920 \times 10^{-3}T$
 317.3-550 K: $\Delta H_r^\circ = -244.508 - 7.909 \times 10^{-3}T + 23.988 \times 10^{-6}T^2 - 31.000T^{-1}$
 $\Delta G_r^\circ = -244.508 + 7.909 \times 10^{-3}T \ln T - 23.988 \times 10^{-6}T^2 - 15.500T^{-1} + 183.575 \times 10^{-3}T$
 550-561 K: $\Delta H_r^\circ = -258.349 - 2.557 \times 10^{-3}T + 23.972 \times 10^{-6}T^2 - 432.200T^{-1}$
 $\Delta G_r^\circ = -258.349 + 2.557 \times 10^{-3}T \ln T - 23.972 \times 10^{-6}T^2 - 216.100T^{-1} + 243.166 \times 10^{-3}T$
 561-787 K: $\Delta H_r^\circ = -286.195 + 79.926 \times 10^{-3}T - 1.616 \times 10^{-6}T^2 - 742.700T^{-1}$
 $\Delta G_r^\circ = -286.195 - 79.926 \times 10^{-3}T \ln T + 1.616 \times 10^{-6}T^2 - 371.350T^{-1} + 801.036 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Vincent (124) and Cueilleron (27) and P(white).
 Low-temperature heat capacities and entropy at 298 K from Clever (21). High-temperature
 data based on Peters (98).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	11.822	21.800	21.800	0	-23.500	-23.097	16.930
300	11.828	21.873	21.800	.022	-23.500	-23.094	16.824
368.3	12.025	24.321	22.048	.837	-23.505	-23.002	13.649
368.3	12.025	24.321	22.048	.837	-23.601	-23.002	13.649
388.36	12.083	24.961	22.182	1.079	-23.609	-22.968	12.925
388.36	12.083	24.961	22.182	1.079	-24.022	-22.968	12.925
400	12.117	25.318	22.268	1.220	-24.045	-22.937	12.532
432.02	12.191	26.254	22.529	1.609	-24.129	-22.845	11.557
500	12.348	28.047	23.161	2.443	-24.424	-22.619	9.887
600	12.556	30.317	24.169	3.689	-24.728	-22.229	8.097
600.65	12.557	30.331	24.175	3.697	-24.729	-22.224	8.086
600.65	12.557	30.331	24.175	3.697	-25.876	-22.224	8.086
700	12.753	32.267	25.190	4.954	-26.136	-21.601	6.744
717.824	12.787	32.588	25.370	5.182	-26.175	-21.484	6.541

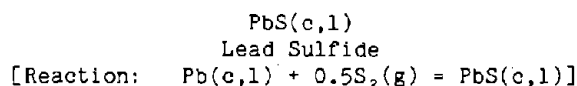
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 600.29 K, melting point of Pb; $\Delta H^\circ = 1.147$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1386.5 K: $\text{Cp}^\circ = 11.534 + 1.806 \times 10^{-3}T - 0.223 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 11.534 \times 10^{-3}T + 0.903 \times 10^{-6}T^2 + 0.223 \times 10^{-2}T^{-1} - 3.594$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta \text{Hf}^\circ = -22.823 - 1.491 \times 10^{-3}T + 0.856 \times 10^{-6}T^2 - 91.900T^{-1}$
 $\Delta \text{Gf}^\circ = -22.823 + 1.491 \times 10^{-3}T \ln T - 0.856 \times 10^{-6}T^2 - 45.950T^{-1} - 8.642 \times 10^{-3}T$
 368.3-388.36 K: $\Delta \text{Hf}^\circ = -23.938 + 0.772 \times 10^{-3}T - 0.890 \times 10^{-6}T^2 + 63.700T^{-1}$
 $\Delta \text{Gf}^\circ = -23.938 + 0.772 \times 10^{-3}T \ln T + 0.890 \times 10^{-6}T^2 + 31.850T^{-1} + 6.541 \times 10^{-3}T$
 388.36-432.02 K: $\Delta \text{Hf}^\circ = -40.097 + 45.512 \times 10^{-3}T - 44.172 \times 10^{-6}T^2 + 1965.900T^{-1}$
 $\Delta \text{Gf}^\circ = -40.097 - 45.512 \times 10^{-3}T \ln T + 44.172 \times 10^{-6}T^2 + 982.950T^{-1} + 291.770 \times 10^{-3}T$
 432.02-600.65 K: $\Delta \text{Hf}^\circ = -49.575 + 41.606 \times 10^{-3}T - 24.360 \times 10^{-6}T^2 + 5192.400T^{-1}$
 $\Delta \text{Gf}^\circ = -49.575 - 41.606 \times 10^{-3}T \ln T + 24.360 \times 10^{-6}T^2 + 2596.200T^{-1} + 289.922 \times 10^{-3}T$
 600.65-717.824 K: $\Delta \text{Hf}^\circ = -49.923 + 39.042 \times 10^{-3}T - 22.383 \times 10^{-6}T^2 + 5209.000T^{-1}$
 $\Delta \text{Gf}^\circ = -49.923 - 39.042 \times 10^{-3}T \ln T + 22.383 \times 10^{-6}T^2 + 2604.500T^{-1} + 275.261 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHr°	ΔGr°	
298.15	11.822	21.800	21.800	0	-38.855	-32.611	23.904
300	11.828	21.873	21.800	.022	-38.852	-32.572	23.728
400	12.117	25.318	22.268	1.220	-38.696	-30.502	16.665
500	12.348	28.047	23.161	2.443	-38.551	-28.472	12.445
600	12.556	30.317	24.169	3.689	-38.423	-26.470	9.642
600.65	12.557	30.331	24.175	3.697	-38.421	-26.455	9.626
600.65	12.557	30.331	24.175	3.697	-39.568	-26.455	9.626
700	12.753	32.267	25.190	4.954	-39.461	-24.296	7.585
800	12.944	33.983	26.184	6.239	-39.336	-22.135	6.047
900	13.132	35.518	27.137	7.543	-39.183	-19.993	4.855
1000	13.318	36.911	28.046	8.865	-39.011	-17.874	3.906
1100	13.502	38.189	28.911	10.206	-38.817	-15.776	3.134
1200	13.686	39.372	29.734	11.566	-38.597	-13.679	2.491
1300	13.869	40.475	30.518	12.944	-38.361	-11.625	1.954
1386.5	14.026	41.373	31.168	14.150	-38.143	-9.849	1.552
1386.5*	16.000	44.619	31.168	18.650	-33.643	-9.849	1.552
1400	16.000	44.774	31.298	18.866	-33.582	-9.618	1.501
1500	16.000	45.878	32.234	20.466	-33.128	-7.925	1.155
1600	16.000	46.910	33.119	22.066	-32.677	-6.277	.857

*Enthalpy of fusion and heat capacity of liquid estimated.

Phase changes: 600.65 K, melting point of Pb; 1.147 kcal/mol.
1386.5 K, melting point of PbS; $\Delta\text{H}^\circ = 4.5$ kcal/mol.

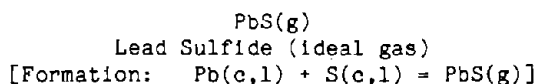
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1386.5 K: $\text{Cp}^\circ = 11.534 + 1.806 \times 10^{-3}\text{T} - 0.223 \times 10^{-5}\text{T}^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 11.534 \times 10^{-3}\text{T} + 0.903 \times 10^{-6}\text{T}^2 + 0.223 \times 10^{-2}\text{T}^{-1} - 3.594$
 1386.5-1600 K: $\text{Cp}^\circ = 16.000$
 $\text{H}^\circ - \text{H}_{298}^\circ = 16.000 \times 10^{-3}\text{T} - 3.534$

Reaction equations (kcal/mol):

298.15-600.65 K: $\Delta\text{Hr}^\circ = -39.612 + 2.512 \times 10^{-3}\text{T} - 1.021 \times 10^{-6}\text{T}^2 + 29.550\text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -39.612 - 2.512 \times 10^{-3}\text{T} \ln \text{T} + 1.021 \times 10^{-6}\text{T}^2 + 14.775\text{T}^{-1} + 37.321 \times 10^{-3}\text{T}$
 600.65-1386.5 K: $\Delta\text{Hr}^\circ = -39.960 - 0.052 \times 10^{-3}\text{T} + 0.956 \times 10^{-6}\text{T}^2 + 46.150\text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -39.960 + 0.052 \times 10^{-3}\text{T} \ln \text{T} - 0.956 \times 10^{-6}\text{T}^2 + 23.075\text{T}^{-1} + 22.660 \times 10^{-3}\text{T}$
 1386.5-1600 K: $\Delta\text{Hr}^\circ = -39.900 + 4.414 \times 10^{-3}\text{T} + 0.053 \times 10^{-6}\text{T}^2 + 23.850\text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -39.900 - 4.414 \times 10^{-3}\text{T} \ln \text{T} - 0.053 \times 10^{-6}\text{T}^2 + 11.925\text{T}^{-1} + 53.681 \times 10^{-3}\text{T}$

Sources: Enthalpy of formation at 298 K based on Kiukkola (69) and Thompson (117). Low-temperature heat capacities and entropy at 298 K based on Anderson (3), Parkinson (95), and Kelley (63). High-temperature data based on Thompson (116) and Blachnik (11). Temperature and enthalpy of fusion and heat capacity of liquid are those estimated by Chase (18).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	8.385	60.062	60.062	0	31.500	20.495	-15.023
300	8.391	60.114	60.062	.016	31.494	20.427	-14.881
368.3	8.549	61.854	60.239	.595	31.252	17.932	-10.641
368.3	8.549	61.854	60.239	.595	31.156	17.932	-10.641
388.36	8.595	62.309	60.334	.767	31.079	17.215	-9.688
388.36	8.595	62.309	60.334	.767	30.666	17.215	-9.688
400	8.622	62.563	60.396	.867	30.602	16.812	-9.186
432.02	8.662	63.228	60.581	1.144	30.405	15.716	-7.950
500	8.746	64.501	61.029	1.736	29.869	13.447	-5.878
600	8.822	66.103	61.745	2.615	29.198	10.225	-3.725
600.65	8.822	66.113	61.749	2.621	29.194	10.207	-3.714
600.65	8.822	66.113	61.749	2.621	28.047	10.207	-3.714
700	8.872	67.467	62.467	3.500	27.410	7.305	-2.281
717.824	8.878	67.690	62.594	3.658	27.302	6.795	-2.069

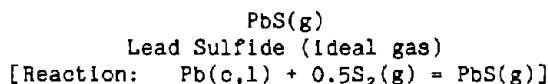
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 600.29 K, melting point of Pb; ΔH° = 1.147 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 8.880 + 0.116x10⁻³T - 0.471x10⁻⁵T²
 H°- H₂₉₈° = 8.880x10⁻³T + 0.058x10⁻⁶T² + 0.471x10⁻²T³ - 2.811

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 32.960 - 4.145x10⁻³T + 0.011x10⁻⁶T² - 67.100T⁻¹
 ΔGf° = 32.960 + 4.145x10⁻³TlnT - 0.011x10⁻⁶T² - 33.550T⁻¹ - 65.043x10⁻³T
 368.3-388.36 K: ΔHf° = 31.845 - 1.882x10⁻³T - 1.735x10⁻⁶T² + 88.500T⁻¹
 ΔGf° = 31.845 + 1.882x10⁻³TlnT + 1.735x10⁻⁶T² + 44.250T⁻¹ - 49.860x10⁻³T
 388.36-432.02 K: ΔHf° = 15.686 + 42.858x10⁻³T - 45.017x10⁻⁶T² + 1990.700T⁻¹
 ΔGf° = 15.686 - 42.858x10⁻³TlnT + 45.017x10⁻⁶T² + 995.350T⁻¹ + 235.368x10⁻³T
 432.02-600.65 K: ΔHf° = 6.208 + 38.952x10⁻³T - 25.205x10⁻⁶T² + 5217.200T⁻¹
 ΔGf° = 6.208 - 38.952x10⁻³TlnT + 25.205x10⁻⁶T² + 2608.600T⁻¹ + 233.520x10⁻³T
 600.65-717.824 K: ΔHf° = 5.860 + 36.388x10⁻³T - 23.228x10⁻⁶T² + 5233.800T⁻¹
 ΔGf° = 5.860 - 36.388x10⁻³TlnT + 23.228x10⁻⁶T² + 2616.900T⁻¹ + 218.859x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	8.385	60.062	60.062	0	16.145	10.981	-8.049
300	8.391	60.114	60.062	.016	16.142	10.950	-7.977
400	8.622	62.563	60.396	.867	15.951	9.247	-5.052
500	8.746	64.501	61.029	1.736	15.742	7.594	-3.319
600	8.822	66.103	61.745	2.615	15.504	5.985	-2.180
600.65	8.822	66.113	61.749	2.621	15.502	5.976	-2.174
600.65	8.822	66.113	61.749	2.621	14.355	5.976	-2.174
700	8.872	67.467	62.467	3.500	14.085	4.610	-1.439
800	8.908	68.654	63.168	4.389	13.814	3.278	-.896
900	8.935	69.705	63.837	5.281	13.555	1.977	-.480
1000	8.957	70.648	64.472	6.176	13.300	.700	-.153
1100	8.975	71.502	65.072	7.073	13.051	-.553	.110
1200	8.991	72.284	65.641	7.971	12.808	-1.768	.322
1300	9.005	73.004	66.180	8.871	12.566	-2.986	.502
1400	9.018	73.672	66.692	9.772	12.324	-4.169	.651
1500	9.031	74.295	67.179	10.674	12.080	-5.343	.778
1600	9.043	74.878	67.642	11.578	11.835	-6.514	.890
1700	9.056	75.427	68.084	12.483	11.587	-7.628	.981
1800	9.069	75.945	68.507	13.389	11.336	-8.752	1.063
1900	9.084	76.435	68.910	14.297	11.085	-9.860	1.134
2000	9.101	76.902	69.299	15.206	10.832	-10.958	1.197

Phase change: 600.65 K, melting point of Pb; 1.147 kcal/mol.

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

298.15-2000 K: $\text{Cp}^\circ = 8.880 + 0.116 \times 10^{-3}T - 0.471 \times 10^{-5}T^{-2}$
 $\text{H}^\circ - \text{H}_{298}^\circ = 8.880 \times 10^{-3}T + 0.058 \times 10^{-6}T^2 + 0.471 \times 10^{-2}T^{-1} - 2.811$

Reaction equations (kcal/mol):

298.15-600.65 K: $\Delta\text{Hr}^\circ = 16.171 - 0.142 \times 10^{-3}T - 1.866 \times 10^{-6}T^2 + 54.350T^{-1}$
 $\Delta\text{Gr}^\circ = 16.171 + 0.142 \times 10^{-3}T \ln T + 1.866 \times 10^{-6}T^2 + 27.175T^{-1} - 19.080 \times 10^{-3}T$
600.65-2000 K: $\Delta\text{Hr}^\circ = 15.823 - 2.706 \times 10^{-3}T + 0.111 \times 10^{-6}T^2 + 70.950T^{-1}$
 $\Delta\text{Gr}^\circ = 15.823 + 2.706 \times 10^{-3}T \ln T - 0.111 \times 10^{-6}T^2 + 35.475T^{-1} - 33.741 \times 10^{-3}T$

Source: Data from Chase (18).

Pd₄S(c)
Tetrapalladium Sulfide
[Formation: 4Pd(c) + S(c,l) = Pd₄S(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	27.470	43.180	43.180	0	-16.500	-16.341	11.978
300*	27.500	43.350	43.180	.051	-16.503	-16.338	11.902
368.3	28.292	49.079	43.756	1.960	-16.687	-16.283	9.662
368.3	28.292	49.079	43.756	1.960	-16.783	-16.283	9.662
388.36	28.525	50.586	44.071	2.530	-16.839	-16.254	9.147
388.36	28.525	50.586	44.071	2.530	-17.252	-16.254	9.147
400	28.660	51.430	44.272	2.863	-17.303	-16.223	8.864
432.02	29.035	53.651	44.886	3.787	-17.460	-16.132	8.160
500	29.830	57.960	46.386	5.787	-17.888	-15.889	6.945
600	31.000	63.500	48.785	8.829	-18.335	-15.447	5.626
700	32.160	68.360	51.237	11.986	-18.662	-14.935	4.663
717.824	32.368	69.171	51.672	12.561	-18.708	-14.839	4.518

*Data above 298 K estimated.

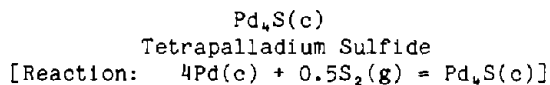
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1000 K: Cp° = 24.156 + 11.468x10⁻³T - 0.094x10⁻⁵T⁻²
H° - H°₂₉₈ = 24.156x10⁻³T + 5.734x10⁻⁶T² + 0.094x10⁻²T⁻¹ - 7.743

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -14.115 - 7.506x10⁻³T + 4.847x10⁻⁶T² - 172.200T⁻¹
ΔGf° = -14.115 + 7.506x10⁻³TlnT - 4.847x10⁻⁶T² - 86.100T⁻¹ - 47.817x10⁻³T
368.3-388.36 K: ΔHf° = -15.231 - 5.243x10⁻³T + 3.101x10⁻⁶T² - 16.600T⁻¹
ΔGf° = -15.231 + 5.243x10⁻³TlnT - 3.101x10⁻⁶T² - 8.300T⁻¹ - 32.635x10⁻³T
388.36-432.02 K: ΔHf° = -31.389 + 39.497x10⁻³T - 40.181x10⁻⁶T² + 1885.600T⁻¹
ΔGf° = -31.389 - 39.497x10⁻³TlnT + 40.181x10⁻⁶T² + 942.800T⁻¹ + 252.594x10⁻³T
432.02-717.824 K: ΔHf° = -40.867 + 35.591x10⁻³T - 20.369x10⁻⁶T² + 5112.100T⁻¹
ΔGf° = -40.867 - 35.591x10⁻³TlnT + 20.369x10⁻⁶T² + 2556.050T⁻¹ + 250.746x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	27.470	43.180	43.180	0	-31.855	-25.855	18.952
300*	27.500	43.350	43.180	.051	-31.855	-25.816	18.806
400	28.660	51.430	44.272	2.863	-31.954	-23.789	12.998
500	29.830	57.960	46.386	5.787	-32.015	-21.743	9.504
600	31.000	63.500	48.785	8.829	-32.029	-19.687	7.171
700	32.160	68.360	51.237	11.986	-31.987	-17.630	5.504
800	33.330	72.730	53.654	15.261	-31.884	-15.585	4.257
900	34.490	76.730	56.006	18.652	-31.716	-13.559	3.293
1000	35.660	80.420	58.260	22.160	-31.492	-11.551	2.525

*Data above 298 K estimated.

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

298.15-1000 K: $C_p^\circ = 24.156 + 11.468 \times 10^{-3}T - 0.094 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 24.156 \times 10^{-3}T + 5.734 \times 10^{-6}T^2 + 0.094 \times 10^{-2}T^3 - 7.743$

Reaction equations (kcal/mol):

298.15-1000 K: $\Delta H_r^\circ = -30.904 - 3.503 \times 10^{-3}T + 2.970 \times 10^{-6}T^2 - 50.750T^{-1}$
 $\Delta G_r^\circ = -30.904 + 3.503 \times 10^{-3}T \ln T - 2.970 \times 10^{-6}T^2 - 25.375T^{-1} - 1.854 \times 10^{-3}T$

Source: Data from Mills (80) who estimated all above 298 K.

PrS(c)
Praseodymium Monosulfide
[Formation: $\text{Pr(c)} + \text{S(c,l)} = \text{PrS(c)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	12.060	20.410	20.410	0	-107.000	-105.533	77.357
300*	12.080	20.480	20.410	.022	-107.000	-105.523	76.872
368.3	12.442	23.006	20.663	.863	-106.996	-105.187	62.417
368.3	12.442	23.006	20.663	.863	-107.092	-105.187	62.417
388.36	12.548	23.669	20.801	1.114	-107.096	-105.082	59.134
388.36	12.548	23.669	20.801	1.114	-107.509	-105.082	59.134
400	12.610	24.040	20.890	1.260	-107.529	-105.009	57.374
432.02	12.709	25.015	21.160	1.665	-107.606	-104.805	53.018
500	12.920	26.890	21.814	2.538	-107.882	-104.338	45.606
600	13.130	29.270	22.868	3.841	-108.166	-103.611	37.740
700	13.300	31.300	23.926	5.162	-108.423	-102.826	32.103
717.824	13.325	31.635	24.113	5.399	-108.466	-102.682	31.263

*Data extrapolated above 298 K.

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2500 K: $C_p^\circ = 12.780 + 1.002 \times 10^{-3}T - 0.906 \times 10^{-5}T^2$
 $H^\circ - H^\circ_{298} = 12.780 \times 10^{-3}T + 0.501 \times 10^{-6}T^2 + 0.906 \times 10^{-2}T^{-1} - 4.159$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -107.112 + 0.436 \times 10^{-3}T - 0.445 \times 10^{-6}T^2 + 6.300T^{-1}$
 $\Delta G_f^\circ = -107.112 - 0.436 \times 10^{-3}T \ln T + 0.445 \times 10^{-6}T^2 + 3.150T^{-1} + 7.611 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -108.227 + 2.699 \times 10^{-3}T - 2.191 \times 10^{-6}T^2 + 161.900T^{-1}$
 $\Delta G_f^\circ = -108.227 - 2.699 \times 10^{-3}T \ln T + 2.191 \times 10^{-6}T^2 + 80.950T^{-1} + 22.794 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -124.385 + 47.439 \times 10^{-3}T - 45.473 \times 10^{-6}T^2 + 2064.100T^{-1}$
 $\Delta G_f^\circ = -124.385 - 47.439 \times 10^{-3}T \ln T + 45.473 \times 10^{-6}T^2 + 1032.050T^{-1} + 308.023 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -133.864 + 43.533 \times 10^{-3}T - 25.661 \times 10^{-6}T^2 + 5290.600T^{-1}$
 $\Delta G_f^\circ = -133.864 - 43.533 \times 10^{-3}T \ln T + 25.661 \times 10^{-6}T^2 + 2645.300T^{-1} + 306.175 \times 10^{-3}T$

PrS(c)
Praseodymium Monosulfide
[Reaction: $\text{Pr(c,l)} + 0.5\text{S}_2(\text{g}) = \text{PrS(c)}$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	12.060	20.410	20.410	0	-122.355	-115.046	84.330
300*	12.080	20.480	20.410	.022	-122.352	-115.000	83.776
400	12.610	24.040	20.890	1.260	-122.180	-112.575	61.507
500	12.920	26.890	21.814	2.538	-122.009	-110.192	48.164
600	13.130	29.270	22.868	3.841	-121.860	-107.852	39.284
700	13.300	31.300	23.926	5.162	-121.748	-105.521	32.945
800	13.440	33.090	24.966	6.499	-121.671	-103.212	28.196
900	13.570	34.680	25.958	7.850	-121.637	-100.900	24.501
1000	13.690	36.110	26.897	9.213	-121.649	-98.591	21.547
1068	13.772	37.013	27.512	10.147	-121.688	-97.028	19.855
1068	13.772	37.013	27.512	10.147	-122.445	-97.028	19.855
1100	13.810	37.420	27.795	10.588	-122.442	-96.267	19.126
1200	13.920	38.630	28.652	11.974	-122.425	-93.892	17.100
1204	13.924	38.676	28.685	12.030	-122.425	-93.790	17.025
1204	13.924	38.676	28.685	12.030	-124.071	-93.790	17.025
1300	14.030	39.750	29.465	13.371	-124.152	-91.378	15.362
1400	14.140	40.790	30.233	14.780	-124.229	-88.849	13.870
1500	14.240	41.770	30.971	16.199	-124.299	-86.319	12.577
1600	14.350	42.690	31.672	17.628	-124.363	-83.787	11.445
1700	14.450	43.570	32.354	19.068	-124.420	-81.249	10.445
1800	14.560	44.400	33.001	20.519	-124.468	-78.721	9.558
1900	14.660	45.190	33.622	21.980	-124.509	-76.170	8.761
2000	14.760	45.940	34.215	23.451	-124.544	-73.609	8.044

*Data extrapolated 300 to 1300 K.

Phase changes: 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:

298.15-2500 K: $\text{Cp}^\circ = 12.780 + 1.002 \times 10^{-3}T - 0.906 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 12.780 \times 10^{-3}T + 0.501 \times 10^{-6}T^2 + 0.906 \times 10^{-2}T^3 - 4.159$

Reaction equations (kcal/mol):

298.15-1068 K: $\Delta\text{Hr}^\circ = -123.900 + 4.438 \times 10^{-3}T - 2.322 \times 10^{-6}T^2 + 127.750T^{-1}$
 $\Delta\text{Gr}^\circ = -123.900 - 4.438 \times 10^{-3}T \ln T + 2.322 \times 10^{-6}T^2 + 63.875T^{-1} + 53.574 \times 10^{-3}T$
1068-1204 K: $\Delta\text{Hr}^\circ = -122.267 - 0.582 \times 10^{-3}T + 0.341 \times 10^{-6}T^2 + 56.450T^{-1}$
 $\Delta\text{Gr}^\circ = -122.267 + 0.582 \times 10^{-3}T \ln T - 0.341 \times 10^{-6}T^2 + 28.225T^{-1} + 19.913 \times 10^{-3}T$
1204-2000 K: $\Delta\text{Hr}^\circ = -122.612 - 1.662 \times 10^{-3}T + 0.341 \times 10^{-6}T^2 + 56.450T^{-1}$
 $\Delta\text{Gr}^\circ = -122.612 + 1.662 \times 10^{-3}T \ln T - 0.341 \times 10^{-6}T^2 + 28.225T^{-1} + 12.539 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Cater (14). Low-temperature heat capacities and entropy at 298 K from Vasilev (123). High-temperature data based on Fesenko (38). Data extrapolated from 300 to 1300 K.

PrS(g)
Praseodymium Monosulfide (ideal gas)
[Formation: $\text{Pr(c)} + \text{S(c,l)} = \text{PrS(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	8.200	62.680	62.680	0	33.000	21.864	-16.027
300	8.210	62.730	62.680	.015	32.993	21.795	-15.878
368.3	8.415	64.441	62.854	.585	32.726	19.274	-11.437
368.3	8.415	64.441	62.854	.585	32.630	19.274	-11.437
388.36	8.475	64.889	62.947	.754	32.545	18.550	-10.439
388.36	8.475	64.889	62.947	.754	32.132	18.550	-10.439
400	8.510	65.140	63.007	.853	32.064	18.144	-9.913
432.02	8.555	65.797	63.190	1.126	31.855	17.037	-8.618
500	8.650	67.050	63.626	1.712	31.292	14.756	-6.450
600	8.730	68.640	64.338	2.581	30.574	11.507	-4.191
700	8.780	69.990	65.053	3.456	29.871	8.385	-2.618
717.824	8.785	70.211	65.178	3.613	29.747	7.840	-2.387

*Data except enthalpy of formation at 298 K estimated.

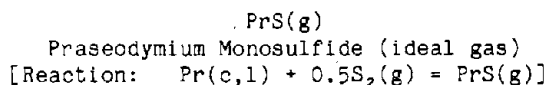
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2500 K: $C_p^\circ = 8.875 + 0.036 \times 10^{-3}T - 0.608 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 8.875 \times 10^{-3}T + 0.018 \times 10^{-6}T^2 + 0.608 \times 10^{-2}T^{-1} - 2.852$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 34.196 - 3.469 \times 10^{-3}T - 0.928 \times 10^{-6}T^2 - 23.500T^{-1}$
 $\Delta G_f^\circ = 34.196 + 3.469 \times 10^{-3}T \ln T + 0.928 \times 10^{-6}T^2 - 11.750T^{-1} - 61.269 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = 33.080 - 1.206 \times 10^{-3}T - 2.674 \times 10^{-6}T^2 + 132.100T^{-1}$
 $\Delta G_f^\circ = 33.080 + 1.206 \times 10^{-3}T \ln T + 2.674 \times 10^{-6}T^2 + 66.050T^{-1} - 46.086 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = 16.922 + 43.534 \times 10^{-3}T - 45.956 \times 10^{-6}T^2 + 2034.300T^{-1}$
 $\Delta G_f^\circ = 16.922 - 43.534 \times 10^{-3}T \ln T + 45.956 \times 10^{-6}T^2 + 1017.150T^{-1} + 239.143 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = 7.443 + 39.628 \times 10^{-3}T - 26.144 \times 10^{-6}T^2 + 5260.800T^{-1}$
 $\Delta G_f^\circ = 7.443 - 39.628 \times 10^{-3}T \ln T + 26.144 \times 10^{-6}T^2 + 2630.400T^{-1} + 237.295 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	8.200	62.680	62.680	0	17.645	12.351	-9.053
300	8.210	62.730	62.680	.015	17.641	12.318	-8.974
400	8.510	65.140	63.007	.853	17.413	10.578	-5.779
500	8.650	67.050	63.626	1.712	17.165	8.902	-3.891
600	8.730	68.640	64.338	2.581	16.880	7.266	-2.647
700	8.780	69.990	65.053	3.456	16.546	5.690	-1.776
800	8.810	71.160	65.741	4.335	16.165	4.168	-1.139
900	8.830	72.200	66.403	5.217	15.730	2.699	-.655
1000	8.850	73.130	67.028	6.102	15.240	1.279	-.279
1068	8.857	73.718	67.442	6.704	14.869	.327	-.067
1068	8.857	73.718	67.442	6.704	14.112	.327	-.067
1100	8.860	73.980	67.628	6.987	13.957	-.084	.017
1200	8.880	74.750	68.188	7.874	13.475	-1.336	.243
1204	8.880	74.780	68.210	7.910	13.455	-1.379	.250
1204	8.880	74.780	68.210	7.910	11.809	-1.379	.250
1300	8.880	75.460	68.720	8.762	11.239	-2.410	.405
1400	8.890	76.120	69.226	9.651	10.643	-3.440	.537
1500	8.900	76.730	69.703	10.541	10.043	-4.417	.644
1600	8.910	77.310	70.165	11.432	9.441	-5.375	.734
1700	8.910	77.850	70.601	12.323	8.836	-6.270	.806
1800	8.920	78.360	71.019	13.214	8.228	-7.154	.869
1900	8.930	78.840	71.415	14.107	7.618	-7.978	.918
2000	8.930	79.300	71.800	15.000	7.006	-8.780	.959

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 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:

298.15-2500 K: $\text{Cp}^\circ = 8.875 + 0.036 \times 10^{-3}T - 0.608 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 8.875 \times 10^{-3}T + 0.018 \times 10^{-6}T^2 + 0.608 \times 10^{-2}T^{-1} - 2.852$

Reaction equations (kcal/mol):

298.15-1068 K: $\Delta \text{Hr}^\circ = 17.407 + 0.533 \times 10^{-3}T - 2.805 \times 10^{-6}T^2 + 97.950T^{-1}$
 $\Delta \text{Gr}^\circ = 17.407 - 0.533 \times 10^{-3}T \ln T + 2.805 \times 10^{-6}T^2 + 48.975T^{-1} - 15.306 \times 10^{-3}T$
1068-1204 K: $\Delta \text{Hr}^\circ = 19.040 - 4.486 \times 10^{-3}T - 0.142 \times 10^{-6}T^2 + 26.650T^{-1}$
 $\Delta \text{Gr}^\circ = 19.040 + 4.486 \times 10^{-3}T \ln T + 0.142 \times 10^{-6}T^2 + 13.325T^{-1} - 48.967 \times 10^{-3}T$
1204-2000 K: $\Delta \text{Hr}^\circ = 18.695 - 5.567 \times 10^{-3}T - 0.142 \times 10^{-6}T^2 + 26.650T^{-1}$
 $\Delta \text{Gr}^\circ = 18.695 + 5.567 \times 10^{-3}T \ln T + 0.142 \times 10^{-6}T^2 + 13.325T^{-1} - 56.341 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Cater (14). Other data are those estimated by Mills (80).

Pr₃S₄(c)
 Tripraseodymium Tetrasulfide
 [Formation: 3Pr(c) + 4S(c,1) = Pr₃S₄(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15*	42.820	61.200	61.200	0	-371.000	-364.305	267.040
300	42.830	61.460	61.200	.079	-370.997	-364.262	265.361
368.3	43.083	70.278	62.096	3.013	-370.957	-362.736	215.245
368.3	43.083	70.278	62.096	3.013	-371.341	-362.736	215.245
388.36	43.157	72.565	62.578	3.878	-371.358	-362.264	203.862
388.36	43.157	72.565	62.578	3.878	-373.010	-362.264	203.862
400	43.200	73.840	62.887	4.381	-373.096	-361.942	197.753
432.02	43.322	77.171	63.824	5.766	-373.420	-361.039	182.640
500	43.580	83.520	66.080	8.720	-374.587	-358.983	156.909
600	43.960	91.500	69.672	13.097	-375.828	-355.759	129.584
700	44.330	98.300	73.284	17.511	-376.948	-352.319	109.998
717.824	44.398	99.415	73.919	18.302	-377.135	-351.688	107.075

*Data except enthalpy of formation at 298 K estimated.

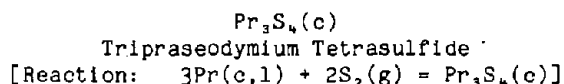
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 41.700 + 3.760x10⁻³T
 H° - H₂₉₈° = 41.700x10⁻³T + 1.880x10⁻⁶T² - 12.600

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -368.652 - 3.506x10⁻³T + 0.759x10⁻⁶T² - 408.500T⁻¹
 ΔGf° = -368.652 + 3.506x10⁻³T lnT - 0.759x10⁻⁶T² - 204.250T⁻¹ - 2.873x10⁻³T
 368.3-388.36 K: ΔHf° = -373.112 + 5.546x10⁻³T - 6.225x10⁻⁶T² + 213.900T⁻¹
 ΔGf° = -373.112 - 5.546x10⁻³T lnT + 6.225x10⁻⁶T² + 106.950T⁻¹ + 57.859x10⁻³T
 388.36-432.02 K: ΔHf° = -437.746 + 184.506x10⁻³T - 179.353x10⁻⁶T² + 7822.700T⁻¹
 ΔGf° = -437.746 - 184.506x10⁻³T lnT + 179.353x10⁻⁶T² + 3911.350T⁻¹ + 1198.773x10⁻³T
 432.02-717.824 K: ΔHf° = -475.661 + 168.882x10⁻³T - 100.105x10⁻⁶T² + 20728.700T⁻¹
 ΔGf° = -475.661 - 168.882x10⁻³T lnT + 100.105x10⁻⁶T² + 10364.350T⁻¹ + 1191.383x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	42.820	61.200	61.200	0	-432.420	-402.360	294.934
300	42.830	61.460	61.200	.079	-432.405	-402.171	292.978
400	43.200	73.840	62.887	4.381	-431.700	-392.204	214.288
500	43.580	83.520	66.080	8.720	-431.097	-382.396	167.143
600	43.960	91.500	69.672	13.097	-430.606	-372.723	135.762
700	44.330	98.300	73.284	17.511	-430.248	-363.100	113.363
800	44.710	104.240	76.786	21.963	-430.010	-353.519	96.576
900	45.080	109.530	80.138	26.453	-429.911	-343.948	83.521
1000	45.460	114.300	83.320	30.980	-429.954	-334.400	73.082
1068	45.718	117.298	85.388	34.080	-430.077	-327.919	67.103
1068	45.718	117.298	85.388	34.080	-432.348	-327.919	67.103
1100	45.840	118.650	86.336	35.545	-432.339	-324.792	64.529
1200	46.210	122.660	89.204	40.147	-432.298	-315.022	57.373
1204	46.225	122.814	89.316	40.332	-432.297	-314.610	57.107
1204	46.225	122.814	89.316	40.332	-437.235	-314.610	57.107
1300	46.590	126.370	91.918	44.787	-437.483	-304.826	51.245
1400	46.960	129.840	94.508	49.465	-437.720	-294.620	45.992
1500	47.340	133.090	96.970	54.180	-437.934	-284.382	41.434
1600	47.720	136.160	99.327	58.933	-438.127	-274.159	37.448
1700	48.090	139.060	101.576	63.723	-438.296	-263.862	33.921
1800	48.470	141.820	103.736	68.551	-438.437	-253.635	30.795
1900	48.840	144.450	105.809	73.417	-438.554	-243.337	27.990
2000	49.220	146.970	107.810	78.320	-438.646	-233.050	25.466

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 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:

298.15-2000 K: Cp° = 41.700 + 3.760x10⁻³T
 H° - H₂₉₈° = 41.700x10⁻³T + 1.880x10⁻⁶T² - 12.600

Reaction equations (kcal/mol):

298.15-1068 K: ΔHr° = -435.807 + 12.504x10⁻³T - 6.749x10⁻⁶T² + 77.300T⁻¹
 ΔGr° = -435.807 - 12.504x10⁻³T lnT + 6.749x10⁻⁶T² + 38.650T⁻¹ + 180.979x10⁻³T
 1068-1204 K: ΔHr° = -430.906 - 2.556x10⁻³T + 1.240x10⁻⁶T² - 136.600T⁻¹
 ΔGr° = -430.906 + 2.556x10⁻³T lnT - 1.240x10⁻⁶T² - 68.300T⁻¹ + 79.995x10⁻³T
 1204-2000 K: ΔHr° = -431.943 - 5.796x10⁻³T + 1.240x10⁻⁶T² - 136.600T⁻¹
 ΔGr° = -431.943 + 5.796x10⁻³T lnT - 1.240x10⁻⁶T² - 68.300T⁻¹ + 57.873x10⁻³T

Source: Data from Mills (80) who estimated all except enthalpy of formation at 298 K.

PtS(c)
Platinum Monosulfide
[Formation: Pt(c) + S(c,l) = PtS(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°-H ₂₉₈ °)/T	H°-H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	10.370	13.160	13.160	0	-19.900	-18.573	13.614
300*	10.390	13.220	13.160	.019	-19.902	-18.563	13.523
368.3	10.916	15.419	13.382	.750	-19.982	-18.253	10.831
368.3	10.916	15.419	13.382	.750	-20.078	-18.253	10.831
388.36	11.070	16.002	13.502	.971	-20.103	-18.152	10.215
388.36	11.070	16.002	13.502	.971	-20.516	-18.152	10.215
400	11.160	16.330	13.580	1.100	-20.548	-18.081	9.879
432.02	11.343	17.196	13.816	1.460	-20.654	-17.880	9.045
500	11.730	18.880	14.388	2.246	-20.977	-17.411	7.610
600	12.230	21.070	15.330	3.444	-21.288	-16.672	6.073
700	12.700	22.990	16.289	4.691	-21.505	-15.883	4.959
717.824	12.778	23.310	16.459	4.918	-21.535	-15.739	4.792

*Data above 298 K estimated.

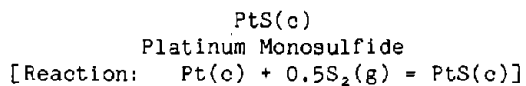
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1500 K: Cp° = 9.985 + 4.098x10⁻³T - 0.744x10⁻⁵T²
 H°-H₂₉₈° = 9.985x10⁻³T + 2.049x10⁻⁶T² + 0.744x10⁻²T⁻¹ - 3.409

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -18.703 - 4.015x10⁻³T + 3.136x10⁻⁶T² - 83.200T⁻¹
 ΔGf° = -18.703 + 4.015x10⁻³TlnT - 3.136x10⁻⁶T² - 41.600T⁻¹ - 21.038x10⁻³T
 368.3-388.36 K: ΔHf° = -19.818 - 1.752x10⁻³T + 1.390x10⁻⁶T² + 72.400T⁻¹
 ΔGf° = -19.818 + 1.752x10⁻³TlnT - 1.390x10⁻⁶T² + 36.200T⁻¹ - 5.855x10⁻³T
 388.36-432.02 K: ΔHf° = -35.976 + 42.988x10⁻³T - 41.892x10⁻⁶T² + 1974.600T⁻¹
 ΔGf° = -35.976 - 42.988x10⁻³TlnT + 41.892x10⁻⁶T² + 987.300T⁻¹ + 279.374x10⁻³T
 432.02-717.824 K: ΔHf° = -45.455 + 39.082x10⁻³T - 22.080x10⁻⁶T² + 5201.100T⁻¹
 ΔGf° = -45.455 - 39.082x10⁻³TlnT + 22.080x10⁻⁶T² + 2600.550T⁻¹ + 277.526x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H _{2,98} °)/T	H°- H _{2,98} °	ΔHr°	ΔGr°	
298.15	10.370	13.160	13.160	0	-35.255	-28.087	20.588
300*	10.390	13.220	13.160	.019	-35.254	-28.040	20.427
400	11.160	16.330	13.580	1.100	-35.199	-25.646	14.012
500	11.730	18.880	14.388	2.246	-35.104	-23.265	10.169
600	12.230	21.070	15.330	3.444	-34.982	-20.913	7.617
700	12.700	22.990	16.289	4.691	-34.830	-18.578	5.800
800	13.140	24.710	17.231	5.983	-34.651	-16.265	4.443
900	13.580	26.290	18.157	7.320	-34.443	-13.985	3.396
1000	14.010	27.740	19.041	8.699	-34.208	-11.720	2.561
1100	14.430	29.100	19.899	10.121	-33.948	-9.490	1.885
1200	14.850	30.370	20.716	11.585	-33.661	-7.274	1.325
1300	15.270	31.570	21.500	13.091	-33.351	-5.083	.854
1400	15.690	32.720	22.264	14.639	-33.014	-2.923	.456
1500	16.100	33.820	23.001	16.228	-32.652	-.792	.115

*Data above 298 K estimated.

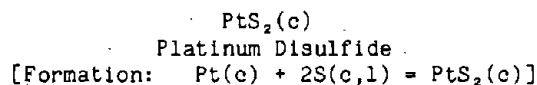
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $C_p^\circ = 9.985 + 4.098 \times 10^{-3}T - 0.744 \times 10^{-5}T^2$
 $H^\circ - H_{2,98}^\circ = 9.985 \times 10^{-3}T + 2.049 \times 10^{-6}T^2 + 0.744 \times 10^{-2}T^{-1} - 3.409$

Reaction equations (kcal/mol):

298.15-1500 K: $\Delta H_r^\circ = -35.491 - 0.013 \times 10^{-3}T + 1.259 \times 10^{-6}T^2 + 38.250T^{-1}$
 $\Delta G_r^\circ = -35.491 + 0.013 \times 10^{-3}T \ln T - 1.259 \times 10^{-6}T^2 + 19.125T^{-1} + 24.925 \times 10^{-3}T$

Source: Data from Mills (80) who estimated all above 298 K.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	15.750	17.850	17.850	0	-26.400	-24.187	17.729
300*	15.780	17.950	17.853	.029	-26.402	-24.174	17.610
368.3	16.559	21.288	18.192	1.140	-26.486	-23.660	14.040
368.3	16.559	21.288	18.192	1.140	-26.678	-23.660	14.040
388.36	16.787	22.172	18.375	1.475	-26.708	-23.494	13.221
388.36	16.787	22.172	18.375	1.475	-27.534	-23.494	13.221
400	16.920	22.670	18.493	1.671	-27.587	-23.372	12.770
432.02	17.154	23.982	18.851	2.217	-27.771	-23.029	11.650
500	17.650	26.520	19.718	3.401	-28.369	-22.225	9.714
600	18.220	29.790	21.132	5.195	-28.941	-20.940	7.627
700	18.710	32.640	22.580	7.042	-29.358	-19.574	6.111
717.824	18.790	33.111	22.836	7.376	-29.417	-19.323	5.883

*Data above 298 K estimated.

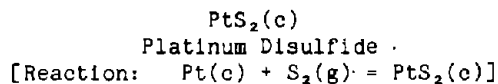
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1500 K: Cp° = 16.405 + 3.756x10⁻³T - 1.578x10⁻⁵T²
H°- H₂₉₈° = 16.405x10⁻³T + 1.878x10⁻⁶T² + 1.578x10⁻²T³ - 5.587

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -24.575 - 5.769x10⁻³T + 4.682x10⁻⁶T² - 155.400T⁻¹
ΔGf° = -24.575 + 5.769x10⁻³TlnT - 4.682x10⁻⁶T² - 77.700T⁻¹ - 29.299x10⁻³T
368.3-388.36 K: ΔHf° = -26.805 - 1.243x10⁻³T + 1.190x10⁻⁶T² + 155.800T⁻¹
ΔGf° = -26.805 + 1.243x10⁻³TlnT - 1.190x10⁻⁶T² + 77.900T⁻¹ + 1.067x10⁻³T
388.36-432.02 K: ΔHf° = -59.122 + 88.237x10⁻³T - 85.374x10⁻⁶T² + 3960.200T⁻¹
ΔGf° = -59.122 - 88.237x10⁻³TlnT + 85.374x10⁻⁶T² + 1980.100T⁻¹ + 571.524x10⁻³T
432.02-717.824 K: ΔHf° = -78.079 + 80.425x10⁻³T - 45.750x10⁻⁶T² + 10413.200T⁻¹
ΔGf° = -78.079 - 80.425x10⁻³TlnT + 45.750x10⁻⁶T² + 5206.600T⁻¹ + 567.829x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	C _p ^o	S ^o	-(G ^o - H ₂₉₈ ^o)/T	H ^o - H ₂₉₈ ^o	ΔH _r ^o	ΔG _r ^o	
298.15	15.750	17.850	17.850	0	-57.110	-43.214	31.677
300*	15.780	17.950	17.853	.029	-57.106	-43.128	31.418
400	16.920	22.670	18.493	1.671	-56.889	-38.503	21.037
500	17.650	26.520	19.718	3.401	-56.624	-33.932	14.831
600	18.220	29.790	21.132	5.195	-56.330	-29.422	10.717
700	18.710	32.640	22.580	7.042	-56.008	-24.964	7.794
800	19.160	35.170	24.000	8.936	-55.662	-20.554	5.615
900	19.590	37.450	25.369	10.873	-55.294	-16.187	3.931
1000	20	39.530	26.677	12.853	-54.902	-11.856	2.591
1100	20.410	41.460	27.938	14.874	-54.490	-7.576	1.505
1200	20.800	43.250	29.138	16.934	-54.059	-3.327	.606
1300	21.200	44.930	30.288	19.034	-53.609	.882	-.148
1400	21.590	46.520	31.396	21.174	-53.138	5.052	-.789
1500	21.980	48.020	32.452	23.352	-52.649	9.194	-1.340

*Data above 298 K estimated.

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

298.15-1500 K: $C_p^o = 16.405 + 3.756 \times 10^{-3}T - 1.578 \times 10^{-5}T^2$
 $H^o - H_{298}^o = 16.405 \times 10^{-3}T + 1.878 \times 10^{-6}T^2 + 1.578 \times 10^{-2}T^{-1} - 5.587$

Reaction equations (kcal/mol):

298.15-1500 K: $\Delta H_r^o = -58.153 + 2.236 \times 10^{-3}T + 0.928 \times 10^{-6}T^2 + 87.500T^{-1}$
 $\Delta G_r^o = -58.153 - 2.236 \times 10^{-3}T \ln T - 0.928 \times 10^{-6}T^2 + 43.750T^{-1} + 62.627 \times 10^{-3}T$

Source: Data from Mills (80) who estimated all above 298 K.

PuS(c)
Plutonium Monosulfide
[Formation: Pu(c) + S(c,l) = PuS(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15*	11.550	18.000	18.000	0	-87.000	-86.081	63.099
300	11.560	18.071	18.001	.021	-87.004	-86.076	62.706
368.3	11.854	20.472	18.242	.821	-87.152	-85.850	50.943
368.3	11.854	20.472	18.242	.821	-87.248	-85.850	50.943
388.36	11.940	21.103	18.374	1.060	-87.309	-85.771	48.267
388.36	11.940	21.103	18.374	1.060	-87.722	-85.771	48.267
395	11.969	21.305	18.422	1.139	-87.754	-85.738	47.437
395	11.969	21.305	18.422	1.139	-88.574	-85.738	47.437
400	11.990	21.456	18.458	1.199	-88.593	-85.702	46.825
432.02	12.124	22.384	18.716	1.585	-88.733	-85.466	43.235
480	12.326	23.672	19.148	2.172	-89.031	-85.083	38.739
480	12.326	23.672	19.148	2.172	-89.166	-85.083	38.739
500	12.410	24.177	19.339	2.419	-89.281	-84.911	37.114
588	12.771	26.217	20.218	3.527	-89.709	-84.106	31.260
588	12.771	26.217	20.218	3.527	-89.849	-84.106	31.260
600	12.820	26.476	20.341	3.681	-89.900	-83.988	30.592
700	13.210	28.482	21.365	4.982	-90.287	-82.971	25.904
717.824	13.279	28.815	21.546	5.218	-90.346	-82.784	25.204

*Data estimated.

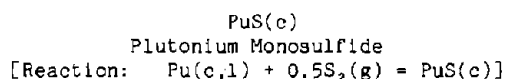
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 395 K, α - β transition point of Pu; ΔH° = 0.820 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 480 K, β - γ transition point of Pu; ΔH° = 0.135 kcal/mol.
 588 K, γ - δ transition point of Pu; ΔH° = 0.140 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 10.909 + 3.396x10⁻³T - 0.330x10⁻⁵T⁻²
 H° - H₂₉₈° = 10.909x10⁻³T + 1.698x10⁻⁶T² + 0.330x10⁻²T⁻¹ - 3.514

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -85.943 - 1.255x10⁻³T - 3.059x10⁻⁶T² - 122.600T⁻¹
 ΔGf° = -85.943 + 1.255x10⁻³TlnT + 3.059x10⁻⁶T² - 61.300T⁻¹ - 7.838x10⁻³T
 368.3-388.36 K: ΔHf° = -87.058 + 1.008x10⁻³T - 4.805x10⁻⁶T² + 33.000T⁻¹
 ΔGf° = -87.058 - 1.008x10⁻³TlnT + 4.805x10⁻⁶T² + 16.500T⁻¹ + 7.345x10⁻³T
 388.36-395 K: ΔHf° = -103.216 + 45.748x10⁻³T - 48.087x10⁻⁶T² + 1935.200T⁻¹
 ΔGf° = -103.216 - 45.748x10⁻³TlnT + 48.087x10⁻⁶T² + 967.600T⁻¹ + 292.573x10⁻³T
 395-432.02 K: ΔHf° = -103.827 + 43.681x10⁻³T - 44.197x10⁻⁶T² + 1935.200T⁻¹
 ΔGf° = -103.827 - 43.681x10⁻³TlnT + 44.197x10⁻⁶T² + 967.600T⁻¹ + 283.297x10⁻³T
 432.02-480 K: ΔHf° = -113.305 + 39.775x10⁻³T - 24.385x10⁻⁶T² + 5161.700T⁻¹
 ΔGf° = -113.305 - 39.775x10⁻³TlnT + 24.385x10⁻⁶T² + 2580.850T⁻¹ + 281.449x10⁻³T
 480-588 K: ΔHf° = -113.701 + 40.730x10⁻³T - 25.243x10⁻⁶T² + 5161.700T⁻¹
 ΔGf° = -113.701 - 40.730x10⁻³TlnT + 25.243x10⁻⁶T² + 2580.850T⁻¹ + 287.758x10⁻³T
 588-717.824 K: ΔHf° = -112.811 + 36.955x10⁻³T - 21.801x10⁻⁶T² + 5161.700T⁻¹
 ΔGf° = -112.811 - 36.955x10⁻³TlnT + 21.801x10⁻⁶T² + 2580.850T⁻¹ + 264.197x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	11.550	18.000	18.000	0	-102.355	-95.595	70.072
300	11.560	18.071	18.001	.021	-102.356	-95.553	69.610
395	11.969	21.305	18.422	1.139	-102.423	-93.392	51.672
395	11.969	21.305	18.422	1.139	-103.243	-93.392	51.672
400	11.990	21.456	18.458	1.199	-103.244	-93.268	50.959
480	12.326	23.672	19.148	2.172	-103.267	-91.270	41.556
480	12.326	23.672	19.148	2.172	-103.402	-91.270	41.556
500	12.410	24.177	19.339	2.419	-103.409	-90.765	39.673
588	12.771	26.217	20.218	3.527	-103.451	-88.537	32.907
588	12.771	26.217	20.218	3.527	-103.591	-88.537	32.907
600	12.820	26.476	20.341	3.681	-103.594	-88.228	32.137
700	13.210	28.482	21.365	4.982	-103.612	-85.666	26.746
730	13.327	29.039	21.669	5.380	-103.610	-84.897	25.416
730	13.327	29.039	21.669	5.380	-103.630	-84.897	25.416
752	13.413	29.435	21.889	5.675	-103.618	-84.332	24.509
752	13.413	29.435	21.889	5.675	-104.058	-84.332	24.509
800	13.600	30.271	22.367	6.323	-104.016	-83.074	22.695
900	13.980	31.895	23.337	7.702	-103.899	-80.464	19.539
913	14.027	32.096	23.461	7.884	-103.882	-80.126	19.180
913	14.027	32.096	23.461	7.884	-104.557	-80.126	19.180
1000	14.340	33.387	24.269	9.118	-104.587	-77.796	17.002
1100	14.700	34.771	25.162	10.570	-104.592	-75.117	14.924
1200	15.040	36.064	26.017	12.057	-104.567	-72.437	13.192
1300	15.380	37.282	26.837	13.578	-104.510	-69.764	11.728
1400	15.700	38.433	27.624	15.132	-104.425	-67.092	10.473
1500	16.010	39.527	28.382	16.718	-104.311	-64.429	9.387
1600	16.320	40.570	29.111	18.335	-104.169	-61.774	8.438
1700	16.610	41.568	29.814	19.981	-104.003	-59.130	7.602
1800	16.890	42.526	30.495	21.656	-103.810	-56.497	6.860
1900	17.160	43.446	31.152	23.359	-103.592	-53.874	6.197
2000	17.420	44.333	31.789	25.088	-103.352	-51.263	5.602

*Data 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.

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

298.15-2000 K: $C_p^\circ = 10.909 + 3.396 \times 10^{-3}T - 0.330 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 10.909 \times 10^{-3}T + 1.698 \times 10^{-6}T^2 + 0.330 \times 10^{-2}T^3 - 3.514$

Reaction equations (kcal/mol):

298.15-395 K: $\Delta H_r^\circ = -102.732 + 2.748 \times 10^{-3}T - 4.936 \times 10^{-6}T^2 - 1.150T^{-1}$
 $\Delta G_r^\circ = -102.732 - 2.748 \times 10^{-3}T \ln T + 4.936 \times 10^{-6}T^2 - 0.575T^{-1} + 38.125 \times 10^{-3}T$
 395-480 K: $\Delta H_r^\circ = -103.342 + 0.680 \times 10^{-3}T - 1.046 \times 10^{-6}T^2 - 1.150T^{-1}$
 $\Delta G_r^\circ = -103.342 - 0.680 \times 10^{-3}T \ln T + 1.046 \times 10^{-6}T^2 - 0.575T^{-1} + 28.849 \times 10^{-3}T$
 480-588 K: $\Delta H_r^\circ = -103.738 + 1.636 \times 10^{-3}T + 1.904 \times 10^{-6}T^2 - 1.150T^{-1}$
 $\Delta G_r^\circ = -103.738 - 1.636 \times 10^{-3}T \ln T + 1.904 \times 10^{-6}T^2 - 0.575T^{-1} + 35.157 \times 10^{-3}T$
 588-730 K: $\Delta H_r^\circ = -102.848 - 2.139 \times 10^{-3}T + 1.538 \times 10^{-6}T^2 - 1.150T^{-1}$
 $\Delta G_r^\circ = -102.848 + 2.139 \times 10^{-3}T \ln T - 1.538 \times 10^{-6}T^2 - 0.575T^{-1} + 11.596 \times 10^{-3}T$
 730-752 K: $\Delta H_r^\circ = -103.143 - 1.763 \times 10^{-3}T + 1.538 \times 10^{-6}T^2 - 1.150T^{-1}$
 $\Delta G_r^\circ = -103.143 + 1.763 \times 10^{-3}T \ln T - 1.538 \times 10^{-6}T^2 - 0.575T^{-1} + 14.486 \times 10^{-3}T$
 752-913 K: $\Delta H_r^\circ = -103.785 - 1.494 \times 10^{-3}T + 1.538 \times 10^{-6}T^2 - 1.150T^{-1}$
 $\Delta G_r^\circ = -103.785 + 1.494 \times 10^{-3}T \ln T - 1.538 \times 10^{-6}T^2 - 0.575T^{-1} + 17.114 \times 10^{-3}T$
 913-2000 K: $\Delta H_r^\circ = -102.754 - 3.363 \times 10^{-3}T + 1.538 \times 10^{-6}T^2 - 1.150T^{-1}$
 $\Delta G_r^\circ = -102.754 + 3.363 \times 10^{-3}T \ln T - 1.538 \times 10^{-6}T^2 - 0.575T^{-1} + 3.251 \times 10^{-3}T$

Source: Data are those estimated by Gronvold (47).

PuS_{1.5}(c)
Plutonium Sesquisulfide
[Formation: Pu(c) + 1.5S(c,l) = PuS_{1.5}(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15*	15.340	22.500	22.500	0	-118.000	-117.281	85.968
300	15.350	22.595	22.502	.028	-118.002	-117.277	85.435
368.3	15.644	25.776	22.822	1.088	-118.082	-117.104	69.489
368.3	15.644	25.776	22.822	1.088	-118.226	-117.104	69.489
388.36	15.730	26.608	22.996	1.403	-118.271	-117.041	65.864
388.36	15.730	26.608	22.996	1.403	-118.890	-117.041	65.864
395	15.759	26.875	23.059	1.507	-118.922	-117.009	64.739
395	15.759	26.875	23.059	1.507	-119.742	-117.009	64.739
400	15.780	27.073	23.108	1.586	-119.761	-116.975	63.911
432.02	15.873	28.292	23.448	2.093	-119.912	-116.747	59.059
480	16.012	29.971	24.017	2.858	-120.271	-116.371	52.984
480	16.012	29.971	24.017	2.858	-120.406	-116.371	52.984
500	16.070	30.626	24.268	3.179	-120.545	-116.200	50.790
588	16.290	33.249	25.421	4.602	-121.036	-115.395	42.890
588	16.290	33.249	25.421	4.602	-121.176	-115.395	42.890
600	16.320	33.578	25.581	4.798	-121.235	-115.275	41.988
700	16.560	36.112	26.908	6.443	-121.678	-114.245	35.668
717.824	16.599	36.529	27.141	6.738	-121.746	-114.054	34.725

*Data estimated.

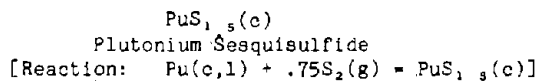
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
395 K, α - β transition point of Pu; ΔH° = 0.820 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
480 K, β - γ transition point of Pu; ΔH° = 0.135 kcal/mol.
588 K, γ - δ transition point of Pu; ΔH° = 0.140 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1500 K: $C_p^\circ = 15.258 + 1.990 \times 10^{-3}T - 0.454 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 15.258 \times 10^{-3}T + 0.995 \times 10^{-6}T^2 + 0.454 \times 10^{-9}T^3 - 4.790$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -116.815 - 0.993 \times 10^{-3}T - 2.903 \times 10^{-6}T^2 - 188.000T^{-1}$
 $\Delta G_f^\circ = -116.815 + 0.993 \times 10^{-3}T \ln T + 2.903 \times 10^{-6}T^2 - 94.000T^{-1} - 7.028 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = -118.488 + 2.401 \times 10^{-3}T - 5.523 \times 10^{-6}T^2 + 45.400T^{-1}$
 $\Delta G_f^\circ = -118.488 - 2.401 \times 10^{-3}T \ln T + 5.523 \times 10^{-6}T^2 + 22.700T^{-1} + 15.746 \times 10^{-3}T$
388.36-395 K: $\Delta H_f^\circ = -142.725 + 69.512 \times 10^{-3}T - 70.446 \times 10^{-6}T^2 + 2898.700T^{-1}$
 $\Delta G_f^\circ = -142.725 - 69.512 \times 10^{-3}T \ln T + 70.446 \times 10^{-6}T^2 + 1449.350T^{-1} + 443.589 \times 10^{-3}T$
395-432.02 K: $\Delta H_f^\circ = -143.336 + 67.444 \times 10^{-3}T - 66.555 \times 10^{-6}T^2 + 2898.700T^{-1}$
 $\Delta G_f^\circ = -143.336 - 67.444 \times 10^{-3}T \ln T + 66.555 \times 10^{-6}T^2 + 1449.350T^{-1} + 434.313 \times 10^{-3}T$
432.02-480 K: $\Delta H_f^\circ = -157.554 + 61.586 \times 10^{-3}T - 36.838 \times 10^{-6}T^2 + 7738.450T^{-1}$
 $\Delta G_f^\circ = -157.554 - 61.586 \times 10^{-3}T \ln T + 36.838 \times 10^{-6}T^2 + 3869.225T^{-1} + 431.541 \times 10^{-3}T$
480-588 K: $\Delta H_f^\circ = -157.950 + 62.541 \times 10^{-3}T - 37.696 \times 10^{-6}T^2 + 7738.450T^{-1}$
 $\Delta G_f^\circ = -157.950 - 62.541 \times 10^{-3}T \ln T + 37.696 \times 10^{-6}T^2 + 3869.225T^{-1} + 437.850 \times 10^{-3}T$
588-717.824 K: $\Delta H_f^\circ = -157.060 + 58.766 \times 10^{-3}T - 34.254 \times 10^{-6}T^2 + 7738.450T^{-1}$
 $\Delta G_f^\circ = -157.060 - 58.766 \times 10^{-3}T \ln T + 34.254 \times 10^{-6}T^2 + 3869.225T^{-1} + 414.289 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	15.340	22.500	22.500	0	-141.033	-131.551	96.429
300	15.350	22.595	22.502	.028	-141.030	-131.493	95.791
395	15.759	26.875	23.059	1.507	-140.925	-128.491	71.092
395	15.759	26.875	23.059	1.507	-141.745	-128.491	71.092
400	15.780	27.073	23.108	1.586	-141.738	-128.324	70.112
480	16.012	29.971	24.017	2.858	-141.626	-125.650	57.209
480	16.012	29.971	24.017	2.858	-141.761	-125.650	57.209
500	16.070	30.626	24.268	3.179	-141.736	-124.980	54.628
588	16.290	33.249	25.421	4.602	-141.650	-122.040	45.360
588	16.290	33.249	25.421	4.602	-141.790	-122.040	45.360
600	16.320	33.578	25.581	4.798	-141.777	-121.637	44.306
700	16.560	36.112	26.908	6.443	-141.665	-118.287	36.931
730	16.626	36.808	27.300	6.941	-141.629	-117.286	35.113
730	16.626	36.808	27.300	6.941	-141.649	-117.286	35.113
752	16.674	37.303	27.586	7.307	-141.613	-116.552	33.873
752	16.674	37.303	27.586	7.307	-142.053	-116.552	33.873
800	16.780	38.338	28.201	8.110	-141.961	-114.928	31.396
900	16.990	40.327	29.440	9.798	-141.756	-111.563	27.091
913	17.017	40.571	29.597	10.019	-141.728	-111.127	26.601
913	17.017	40.571	29.597	10.019	-142.403	-111.127	26.601
1000	17.200	42.128	30.620	11.508	-142.371	-108.146	23.635
1100	17.410	43.777	31.742	13.238	-142.322	-104.727	20.807
1200	17.620	45.301	32.809	14.990	-142.257	-101.311	18.451
1300	17.820	46.719	33.825	16.762	-142.176	-97.903	16.459
1400	18.020	48.047	34.794	18.554	-142.082	-94.500	14.752
1500	18.230	49.297	35.720	20.366	-141.973	-91.105	13.274

*Data 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.

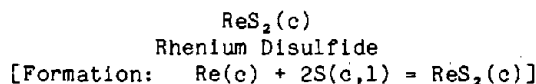
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

$$298.15-1500 \text{ K: } \begin{aligned} \text{Cp}^\circ &= 15.258 + 1.990 \times 10^{-3}T - 0.454 \times 10^{-5}T^2 \\ \text{H}^\circ - \text{H}_{298}^\circ &= 15.258 \times 10^{-3}T + 0.995 \times 10^{-6}T^2 + 0.454 \times 10^{-2}T^{-1} - 4.790 \end{aligned}$$

Reaction equations (kcal/mol):

$$\begin{aligned} 298.15-395 \text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= -141.999 + 5.011 \times 10^{-3}T - 5.719 \times 10^{-6}T^2 - 5.825T^{-1} \\ \Delta \text{Gr}^\circ &= -141.999 - 5.011 \times 10^{-3}T \ln T + 5.719 \times 10^{-6}T^2 - 2.912T^{-1} + 61.917 \times 10^{-3}T \end{aligned} \\ 395-480 \text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= -142.609 + 2.944 \times 10^{-3}T - 1.829 \times 10^{-6}T^2 - 5.825T^{-1} \\ \Delta \text{Gr}^\circ &= -142.609 - 2.944 \times 10^{-3}T \ln T + 1.829 \times 10^{-6}T^2 - 2.912T^{-1} + 52.640 \times 10^{-3}T \end{aligned} \\ 480-588 \text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= -143.005 + 3.899 \times 10^{-3}T - 2.687 \times 10^{-6}T^2 - 5.825T^{-1} \\ \Delta \text{Gr}^\circ &= -143.005 - 3.899 \times 10^{-3}T \ln T + 2.687 \times 10^{-6}T^2 - 2.912T^{-1} + 58.949 \times 10^{-3}T \end{aligned} \\ 588-730 \text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= -142.115 + 0.124 \times 10^{-3}T + 0.755 \times 10^{-6}T^2 - 5.825T^{-1} \\ \Delta \text{Gr}^\circ &= -142.115 - 0.124 \times 10^{-3}T \ln T - 0.755 \times 10^{-6}T^2 - 2.912T^{-1} + 35.387 \times 10^{-3}T \end{aligned} \\ 730-752 \text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= -142.410 + 0.501 \times 10^{-3}T + 0.755 \times 10^{-6}T^2 - 5.825T^{-1} \\ \Delta \text{Gr}^\circ &= -142.410 - 0.501 \times 10^{-3}T \ln T + 0.755 \times 10^{-6}T^2 - 2.912T^{-1} + 38.277 \times 10^{-3}T \end{aligned} \\ 752-913 \text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= -143.052 + 0.769 \times 10^{-3}T + 0.755 \times 10^{-6}T^2 - 5.825T^{-1} \\ \Delta \text{Gr}^\circ &= -143.052 - 0.769 \times 10^{-3}T \ln T - 0.755 \times 10^{-6}T^2 - 2.912T^{-1} + 40.905 \times 10^{-3}T \end{aligned} \\ 913-1500 \text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= -142.021 - 1.099 \times 10^{-3}T + 0.755 \times 10^{-6}T^2 - 5.825T^{-1} \\ \Delta \text{Gr}^\circ &= -142.021 + 1.099 \times 10^{-3}T \ln T - 0.755 \times 10^{-6}T^2 - 2.912T^{-1} + 27.043 \times 10^{-3}T \end{aligned} \end{aligned}$$

Source: Data are those estimated by Gronvold (47).



T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15*	15.750	14.500	14.500	0	-42.700	-39.852	29.212
300	15.780	14.600	14.500	.030	-42.701	-39.834	29.019
368.3	16.559	17.928	14.834	1.139	-42.776	-39.173	23.245
368.3	16.559	17.928	14.834	1.139	-42.968	-39.173	23.245
388.36	16.787	18.812	15.017	1.474	-42.995	-38.965	21.927
388.36	16.787	18.812	15.017	1.474	-43.821	-38.965	21.927
400	16.920	19.310	15.135	1.670	-43.873	-38.819	21.209
432.02	17.154	20.622	15.494	2.216	-44.052	-38.409	19.430
500	17.650	23.170	16.370	3.400	-44.642	-37.469	16.378
600	18.220	26.440	17.790	5.190	-45.204	-35.984	13.107
700	18.710	29.280	19.223	7.040	-45.604	-34.405	10.742
717.824	18.790	29.751	19.478	7.374	-45.661	-34.119	10.388

*Data except enthalpy of formation at 298 K estimated.

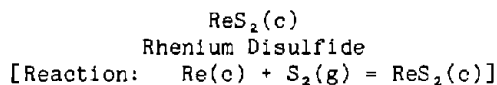
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-1500 K: $C_p^\circ = 16.390 + 3.770 \times 10^{-3}T - 1.570 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 16.390 \times 10^{-3}T + 1.885 \times 10^{-6}T^2 + 1.570 \times 10^{-2}T^{-1} - 5.581$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -40.910 - 5.634 \times 10^{-3}T + 4.673 \times 10^{-6}T^2 - 156.600T^{-1}$
 $\Delta G_f^\circ = -40.910 + 5.634 \times 10^{-3}T \ln T - 4.673 \times 10^{-6}T^2 - 78.300T^{-1} - 26.277 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -43.141 - 1.108 \times 10^{-3}T + 1.181 \times 10^{-6}T^2 + 154.600T^{-1}$
 $\Delta G_f^\circ = -43.141 + 1.108 \times 10^{-3}T \ln T - 1.181 \times 10^{-6}T^2 + 77.300T^{-1} + 4.089 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -75.457 + 88.372 \times 10^{-3}T - 85.383 \times 10^{-6}T^2 + 3959.000T^{-1}$
 $\Delta G_f^\circ = -75.457 - 88.372 \times 10^{-3}T \ln T + 85.383 \times 10^{-6}T^2 + 1979.500T^{-1} + 574.546 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -94.415 + 80.560 \times 10^{-3}T - 45.759 \times 10^{-6}T^2 + 10412.000T^{-1}$
 $\Delta G_f^\circ = -94.415 - 80.560 \times 10^{-3}T \ln T + 45.759 \times 10^{-6}T^2 + 5206.000T^{-1} + 570.851 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15*	15.750	14.500	14.500	0	-73.410	-58.879	43.159
300	15.780	14.600	14.500	.030	-73.405	-58.788	42.827
400	16.920	19.310	15.135	1.670	-73.175	-53.950	29.477
500	17.650	23.170	16.370	3.400	-72.897	-49.176	21.495
600	18.220	26.440	17.790	5.190	-72.593	-44.466	16.196
700	18.710	29.280	19.223	7.040	-72.254	-39.796	12.425
800	19.160	31.810	20.647	8.930	-71.899	-35.188	9.613
900	19.590	34.090	22.012	10.870	-71.516	-30.619	7.435
1000	20	36.180	23.330	12.850	-71.113	-26.100	5.704
1100	20.410	38.100	24.582	14.870	-70.691	-21.613	4.294
1200	20.810	39.890	25.782	16.930	-70.249	-17.168	3.127
1300	21.200	41.580	26.942	19.030	-69.787	-12.777	2.148
1400	21.590	43.160	28.039	21.170	-69.306	-8.400	1.311
1500	21.980	44.660	29.093	23.350	-68.805	-4.062	.592

*Data except enthalpy of formation at 298 K estimated.

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

298.15-1500 K: $C_p^\circ = 16.390 + 3.770 \times 10^{-3}T - 1.570 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 16.390 \times 10^{-3}T + 1.885 \times 10^{-6}T^2 + 1.570 \times 10^{-2}T^{-1} - 5.581$

Reaction equations (kcal/mol):

298.15-1500 K: $\Delta H_r^\circ = -74.488 + 2.371 \times 10^{-3}T + 0.919 \times 10^{-6}T^2 + 86.300T^{-1}$
 $\Delta G_r^\circ = -74.488 - 2.371 \times 10^{-3}T \ln T - 0.919 \times 10^{-6}T^2 + 43.150T^{-1} + 65.649 \times 10^{-3}T$

Source: Data from Mills (80) who estimated all except enthalpy of formation at 298 K.

$\text{Re}_2\text{S}_7(\text{c})$
 Dirhenium Heptasulfide
 [Formation: $2\text{Re}(\text{c}) + 7\text{S}(\text{c,l}) = \text{Re}_2\text{S}_7(\text{c})$]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15*	47.980	40	40	0	-107.900	-98.631	72.298
300	48.000	40.300	40	.090	-107.902	-98.572	71.809
368.3	48.820	50.223	41.002	3.396	-108.117	-96.430	57.221
368.3	48.820	50.223	41.002	3.396	-108.789	-96.430	57.221
388.36	49.060	52.819	41.546	4.378	-108.887	-95.749	53.882
388.36	49.060	52.819	41.546	4.378	-111.778	-95.749	53.882
400	49.200	54.270	41.895	4.950	-111.966	-95.267	52.051
432.02	49.584	58.074	42.955	6.532	-112.623	-93.909	47.506
500	50.400	65.380	45.520	9.930	-114.795	-90.774	39.677
600	51.600	74.670	49.620	15.030	-116.970	-85.752	31.235
700	52.800	82.720	53.791	20.250	-118.650	-80.413	25.106

*Data except enthalpy of formation at 298 K estimated.

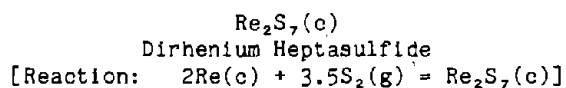
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.

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

298.15-700 K: $C_p^\circ = 44.400 + 12.000 \times 10^{-3} T$
 $H^\circ - H_{298}^\circ = 44.400 \times 10^{-3} T + 6.000 \times 10^{-6} T^2 - 13.771$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -98.511 - 24.170 \times 10^{-3} T + 16.727 \times 10^{-6} T^2 - 1094.000 T^{-1}$
 $\Delta G_f^\circ = -98.511 + 24.170 \times 10^{-3} T \ln T - 16.727 \times 10^{-6} T^2 - 547.000 T^{-1} - 126.973 \times 10^{-3} T$
 368.3-388.36 K: $\Delta H_f^\circ = -106.317 - 8.329 \times 10^{-3} T + 4.505 \times 10^{-6} T^2 - 4.800 T^{-1}$
 $\Delta G_f^\circ = -106.317 + 8.329 \times 10^{-3} T \ln T - 4.505 \times 10^{-6} T^2 - 2.400 T^{-1} - 20.692 \times 10^{-3} T$
 388.36-432.02 K: $\Delta H_f^\circ = -219.425 + 304.851 \times 10^{-3} T - 298.469 \times 10^{-6} T^2 + 13310.600 T^{-1}$
 $\Delta G_f^\circ = -219.425 - 304.851 \times 10^{-3} T \ln T + 298.469 \times 10^{-6} T^2 + 6655.300 T^{-1} + 1975.906 \times 10^{-3} T$
 432.02-700 K: $\Delta H_f^\circ = -285.776 + 277.509 \times 10^{-3} T - 159.785 \times 10^{-6} T^2 + 35896.100 T^{-1}$
 $\Delta G_f^\circ = -285.776 - 277.509 \times 10^{-3} T \ln T + 159.785 \times 10^{-6} T^2 + 17948.050 T^{-1} + 1962.974 \times 10^{-3} T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHr°	ΔGr°	
298.15*	47.980	40	40	0	-215.385	-165.227	121.113
300	48.000	40.300	40	.090	-215.366	-164.913	120.138
400	49.200	54.270	41.895	4.950	-214.523	-148.226	80.986
500	50.400	65.380	45.520	9.930	-213.688	-131.747	57.586
600	51.600	74.670	49.620	15.030	-212.832	-115.438	42.048
700	52.800	82.720	53.791	20.250	-211.925	-99.279	30.996

*Data except enthalpy of formation at 298 K estimated.

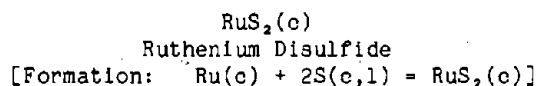
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-700 K: $\text{Cp}^\circ = 44.400 + 12.000 \times 10^{-3} \text{T}$
 $\text{H}^\circ - \text{H}_{298}^\circ = 44.400 \times 10^{-3} \text{T} + 6.000 \times 10^{-6} \text{T}^2 - 13.771$

Reaction equations (kcal/mol):

298.15-700 K: $\Delta\text{Hr}^\circ = -216.033 + 3.848 \times 10^{-3} \text{T} + 3.588 \times 10^{-6} \text{T}^2 - 243.850 \text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -216.033 - 3.848 \times 10^{-3} \text{T} \ln \text{T} - 3.588 \times 10^{-6} \text{T}^2 - 121.925 \text{T}^{-1} + 194.768 \times 10^{-3} \text{T}$

Source: Data from Mills (80) who estimated all except enthalpy of formation at 298 K.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	15.850	13.200	13.200	0	-47.600	-44.928	32.933
300	15.880	13.298	13.201	.029	-47.602	-44.912	32.718
368.3	16.577	16.647	13.537	1.145	-47.653	-44.294	26.284
368.3	16.577	16.647	13.537	1.145	-47.845	-44.294	26.284
388.36	16.782	17.532	13.721	1.480	-47.868	-44.099	24.816
388.36	16.782	17.532	13.721	1.480	-48.694	-44.099	24.816
400	16.901	18.029	13.839	1.676	-48.744	-43.961	24.019
432.02	17.043	19.336	14.199	2.219	-48.921	-43.573	22.042
500	17.344	21.854	15.072	3.391	-49.520	-42.679	18.655
600	17.589	25.040	16.475	5.139	-50.124	-41.249	15.025
700	17.768	27.765	17.898	6.907	-50.614	-39.731	12.404
717.824	17.798	28.212	18.148	7.224	-50.690	-39.452	12.012

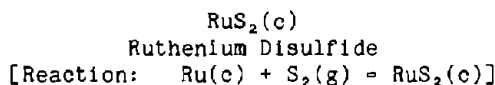
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1500 K: Cp° = 17.012 + 1.618x10⁻³T - 1.462x10⁻⁵T²
H° - H₂₉₈° = 17.012x10⁻³T + 0.809x10⁻⁶T² + 1.462x10⁻²T⁻¹ - 5.634

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -46.203 - 4.043x10⁻³T + 3.039x10⁻⁶T² - 137.800T⁻¹
ΔGf° = -46.203 + 4.043x10⁻³TlnT - 3.039x10⁻⁶T² - 68.900T⁻¹ - 17.080x10⁻³T
368.3-388.36 K: ΔHf° = -48.433 + 0.483x10⁻³T - 0.453x10⁻⁶T² + 173.400T⁻¹
ΔGf° = -48.433 - 0.483x10⁻³TlnT + 0.453x10⁻⁶T² + 86.700T⁻¹ + 13.286x10⁻³T
388.36-432.02 K: ΔHf° = -80.749 + 89.963x10⁻³T - 87.017x10⁻⁶T² + 3977.800T⁻¹
ΔGf° = -80.749 - 89.963x10⁻³TlnT + 87.017x10⁻⁶T² + 1988.900T⁻¹ + 583.742x10⁻³T
432.02-717.824 K: ΔHf° = -99.707 + 82.151x10⁻³T - 47.393x10⁻⁶T² + 10430.800T⁻¹
ΔGf° = -99.707 - 82.151x10⁻³TlnT + 47.393x10⁻⁶T² + 5215.400T⁻¹ + 580.047x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	15.850	13.200	13.200	0	-78.310	-63.956	46.880
300	15.880	13.298	13.201	.029	-78.306	-63.867	46.526
400	16.901	18.029	13.839	1.676	-78.046	-59.092	32.286
500	17.344	21.854	15.072	3.391	-77.775	-54.385	23.771
600	17.589	25.040	16.475	5.139	-77.513	-49.731	18.114
700	17.768	27.765	17.898	6.907	-77.264	-45.121	14.087
800	17.935	30.148	19.283	8.692	-77.025	-40.545	11.076
900	18.117	32.271	20.611	10.494	-76.793	-36.000	8.742
1000	18.327	34.190	21.874	12.316	-76.563	-31.479	6.880
1100	18.573	35.948	23.074	14.161	-76.332	-26.982	5.361
1200	18.860	37.576	24.216	16.032	-76.097	-22.505	4.099
1300	19.190	39.098	25.303	17.934	-75.853	-18.050	3.034
1400	19.567	40.534	26.340	19.872	-75.597	-13.612	2.125
1500	19.990	41.898	27.332	21.849	-75.326	-9.195	1.340

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

298.15-1500 K: $C_p^\circ = 17.012 + 1.618 \times 10^{-3}T - 1.462 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 17.012 \times 10^{-3}T + 0.809 \times 10^{-6}T^2 + 1.462 \times 10^{-2}T^{-1} - 5.634$

Reaction equations (kcal/mol):

298.15-1500 K: $\Delta H_r^\circ = -79.780 + 3.962 \times 10^{-3}T - 0.715 \times 10^{-6}T^2 + 105.100T^{-1}$
 $\Delta G_r^\circ = -79.780 - 3.962 \times 10^{-3}T \ln T + 0.715 \times 10^{-6}T^2 + 52.550T^{-1} + 74.846 \times 10^{-3}T$

Source: Data from Svendsen (114).

S(c,l)

Sulfur

T, K	cal/mol·K			$H^\circ - H_{298}^\circ$, kcal/mol
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	
298.15	5.425	7.661	7.661	0
300	5.436	7.695	7.662	.010
368.3	5.795	8.846	7.776	.394
368.3	5.921	9.106	7.776	.490
388.36	6.015	9.423	7.855	.609
388.36	7.423	10.486	7.854	1.022
400	7.687	10.709	7.934	1.110
432.02	12.860	11.340	8.162	1.373
500	9.078	12.797	8.703	2.047
600	8.200	14.362	9.522	2.904
700	7.799	15.596	10.305	3.704
717.824	7.694	15.790	10.439	3.841

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S;
 $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-368.3 K: $C_p^\circ = 8.174 - 3.434 \times 10^{-3}T - 1.556 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 8.174 \times 10^{-3}T - 1.717 \times 10^{-6}T^2 + 1.556 \times 10^{-2}T^{-1} - 2.806$
 368.3-388.36 K: $C_p^\circ = 5.911 + 0.058 \times 10^{-3}T$
 $H^\circ - H_{298}^\circ = 5.911 \times 10^{-3}T + 0.029 \times 10^{-6}T^2 - 1.691$
 388.36-432.02 K: $C_p^\circ = -38.829 + 86.622 \times 10^{-3}T + 19.022 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = -38.829 \times 10^{-3}T + 43.311 \times 10^{-6}T^2 - 19.022 \times 10^{-2}T^{-1} + 14.467$
 432.02-717.824 K: $C_p^\circ = -34.923 + 46.998 \times 10^{-3}T + 51.287 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = -34.923 \times 10^{-3}T + 23.499 \times 10^{-6}T^2 - 51.287 \times 10^{-2}T^{-1} + 23.946$

Source: Data from Pankratz (91).

S(g)
Sulfur (ideal monatomic gas)
[Formation: S(c,l) = S(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	5.658	40.086	40.086	0	66.200	56.532	-41.439
300	5.657	40.121	40.088	.010	66.200	56.472	-41.139
368.3	5.586	41.275	40.204	.394	66.200	54.257	-32.196
368.3	5.586	41.275	40.204	.394	66.104	54.257	-32.196
388.36	5.565	41.571	40.267	.506	66.097	53.612	-30.170
388.36	5.565	41.571	40.267	.506	65.684	53.612	-30.170
400	5.553	41.735	40.307	.571	65.661	53.251	-29.094
432.02	5.515	42.161	40.429	.748	65.575	52.260	-26.437
500	5.435	42.961	40.719	1.121	65.274	50.192	-21.939
600	5.339	43.943	41.178	1.659	64.955	47.206	-17.195
700	5.266	44.761	41.634	2.189	64.685	44.269	-13.821
717.824	5.256	44.893	41.713	2.283	64.642	43.751	-13.320

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 5.397 - 0.226x10⁻³T + 0.292x10⁵T⁻²
H° - H°₂₉₈ = 5.397x10⁻³T - 0.113x10⁻⁶T² - 0.292x10²T⁻¹ - 1.501

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 67.505 - 2.777x10⁻³T + 1.604x10⁻⁶T² - 184.800T⁻¹
ΔGf° = 67.505 + 2.777x10⁻³T ln T - 1.604x10⁻⁶T² - 92.400T⁻¹ - 51.107x10⁻³T
368.3-388.36 K: ΔHf° = 66.390 - 0.514x10⁻³T - 0.142x10⁻⁶T² - 29.200T⁻¹
ΔGf° = 66.390 + 0.514x10⁻³T ln T + 0.142x10⁻⁶T² - 14.600T⁻¹ - 35.924x10⁻³T
388.36-432.02 K: ΔHf° = 50.232 + 44.226x10⁻³T - 43.424x10⁻⁶T² + 1873.000T⁻¹
ΔGf° = 50.232 - 44.226x10⁻³T ln T + 43.424x10⁻⁶T² + 936.500T⁻¹ + 249.304x10⁻³T
432.02-717.824 K: ΔHf° = 40.753 + 40.320x10⁻³T - 23.612x10⁻⁶T² + 5099.500T⁻¹
ΔGf° = 40.753 - 40.320x10⁻³T ln T + 23.612x10⁻⁶T² + 2549.750T⁻¹ + 247.456x10⁻³T

S(g)
Sulfur (ideal monatomic gas)
[Reaction: $0.5S_2(g) = S(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	5.658	40.086	40.086	0	50.845	47.019	-34.465
300	5.657	40.121	40.088	.010	50.848	46.995	-34.235
400	5.553	41.735	40.307	.571	51.010	45.685	-24.961
500	5.435	42.961	40.719	1.121	51.146	44.339	-19.380
600	5.339	43.943	41.178	1.659	51.260	42.965	-15.650
700	5.266	44.761	41.634	2.189	51.360	41.574	-12.980
800	5.210	45.460	42.069	2.713	51.448	40.171	-10.974
900	5.168	46.071	42.480	3.232	51.528	38.757	-9.411
1000	5.136	46.614	42.867	3.747	51.599	37.333	-8.159
1100	5.111	47.102	43.230	4.259	51.664	35.904	-7.133
1200	5.093	47.546	43.572	4.769	51.722	34.468	-6.277
1300	5.079	47.953	43.893	5.278	51.777	33.028	-5.553
1400	5.069	48.329	44.197	5.785	51.826	31.584	-4.930
1500	5.064	48.679	44.484	6.292	51.870	30.136	-4.391
1600	5.062	49.005	44.756	6.798	51.911	28.687	-3.918
1700	5.063	49.312	45.016	7.304	51.947	27.234	-3.501
1800	5.068	49.602	45.263	7.811	51.982	25.779	-3.130
1900	5.075	49.876	45.498	8.318	52.014	24.322	-2.798
2000	5.085	50.137	45.724	8.826	52.044	22.864	-2.498
2100	5.097	50.385	45.940	9.335	52.071	21.404	-2.228
2200	5.111	50.622	46.147	9.845	52.098	19.944	-1.981
2300	5.127	50.850	46.347	10.357	52.125	18.481	-1.756
2400	5.144	51.068	46.538	10.871	52.151	17.019	-1.550
2500	5.162	51.279	46.725	11.386	52.176	15.554	-1.360
2600	5.181	51.482	46.904	11.903	52.201	14.087	-1.184
2700	5.200	51.678	47.077	12.422	52.228	12.620	-1.022
2800	5.219	51.867	47.244	12.943	52.254	11.155	-.871
2900	5.239	52.050	47.407	13.466	52.282	9.688	-.730
3000	5.258	52.228	47.564	13.991	52.310	8.218	-.599

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

298.15-2000 K: $C_p^\circ = 5.397 - 0.226 \times 10^{-3}T + 0.292 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 5.397 \times 10^{-3}T - 0.113 \times 10^{-6}T^2 - 0.292 \times 10^2 T^{-1} - 1.501$
 2000-3000 K: $C_p^\circ = 4.156 + 0.336 \times 10^{-3}T + 10.352 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 4.156 \times 10^{-3}T + 0.168 \times 10^{-6}T^2 - 10.352 \times 10^2 T^{-1} + 0.360$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = 50.716 + 1.225 \times 10^{-3}T - 0.273 \times 10^{-6}T^2 - 63.350T^{-1}$
 $\Delta G_r^\circ = 50.716 - 1.225 \times 10^{-3}T \ln T + 0.273 \times 10^{-6}T^2 - 31.675T^{-1} - 5.144 \times 10^{-3}T$
 2000-3000 K: $\Delta H_r^\circ = 53.602 - 0.599 \times 10^{-3}T + 0.118 \times 10^{-6}T^2 - 1665.200T^{-1}$
 $\Delta G_r^\circ = 53.602 + 0.599 \times 10^{-3}T \ln T - 0.118 \times 10^{-6}T^2 - 832.600T^{-1} - 19.473 \times 10^{-3}T$

Source: Data from Pankratz (91).



Sulfur (ideal diatomic gas)

T, K	cal/mol·K			H° - H° ₂₉₈
	Cp°	S°	-(G° - H° ₂₉₈)/T	kcal/mol
298.15	7.765	54.506	54.506	0.000
300	7.774	54.555	54.508	0.014
400	8.148	56.845	54.815	0.812
500	8.392	58.691	55.413	1.639
600	8.553	60.236	56.091	2.487
700	8.666	61.563	56.780	3.348
800	8.756	62.727	57.453	4.219
900	8.835	63.762	58.096	5.099
1000	8.909	64.697	58.711	5.986
1100	8.983	65.550	59.295	6.881
1200	9.057	66.335	59.849	7.783
1300	9.131	67.062	60.376	8.692
1400	9.205	67.742	60.878	9.609
1500	9.278	68.379	61.357	10.533
1600	9.348	68.980	61.815	11.464
1700	9.415	69.549	62.253	12.403
1800	9.479	70.089	62.674	13.347
1900	9.539	70.603	63.078	14.298
2000	9.595	71.094	63.467	15.255
2100	9.644	71.563	63.841	16.217
2200	9.691	72.013	64.202	17.184
2300	9.734	72.445	64.552	18.155
2400	9.775	72.860	64.889	19.131
2500	9.812	73.260	65.216	20.110
2600	9.842	73.645	65.532	21.093
2700	9.871	74.017	65.840	22.078
2800	9.898	74.377	66.139	23.067
2900	9.924	74.725	66.429	24.058
3000	9.949	75.061	66.711	25.051

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

$$298.15-2000 \text{ K: } C_p^\circ = 8.343 + 0.640 \times 10^{-3} T - 0.683 \times 10^{-5} T^2$$

$$H^\circ - H_{298}^\circ = 8.343 \times 10^{-3} T + 0.320 \times 10^{-6} T^2 + 0.683 \times 10^{-2} T^{-1} - 2.745$$

$$2000-3000 \text{ K: } C_p^\circ = 9.510 + 0.200 \times 10^{-3} T - 12.600 \times 10^{-5} T^2$$

$$H^\circ - H_{298}^\circ = 9.510 \times 10^{-3} T + 0.100 \times 10^{-6} T^2 + 12.600 \times 10^{-2} T^{-1} - 4.795$$

Source: Data from Pankratz (91).

S₂(g)
Sulfur (ideal diatomic gas)
[Formation: 2S(c,l) = S₂(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H _{2,98} °)/T	H°- H _{2,98} °	ΔHf°	ΔGf°	
298.15	7.765	54.506	54.506	0	30.710	19.027	-13.947
300	7.774	54.555	54.508	.014	30.704	18.954	-13.808
368.3	8.029	56.177	54.669	.556	30.478	16.303	-9.674
368.3	8.029	56.177	54.669	.556	30.286	16.303	-9.674
388.36	8.104	56.605	54.758	.717	30.209	15.545	-8.748
388.36	8.104	56.605	54.758	.717	29.383	15.545	-8.748
400	8.148	56.845	54.815	.812	29.302	15.131	-8.267
432.02	8.226	57.475	54.989	1.074	29.038	14.006	-7.085
500	8.392	58.691	55.413	1.639	28.255	11.706	-5.117
600	8.553	60.236	56.091	2.487	27.389	8.482	-3.089
700	8.666	61.563	56.780	3.348	26.650	5.390	-1.683
717.824	8.682	61.781	56.902	3.503	26.531	4.852	-1.477

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 8.343 + 0.640x10⁻³T - 0.683x10⁻⁵T²
H°- H_{2,98}° = 8.343x10⁻³T + 0.320x10⁻⁶T² + 0.683x10⁻²T⁻¹ - 2.745

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 33.578 - 8.005x10⁻³T + 3.754x10⁻⁶T² - 242.900T⁻¹
ΔGf° = 33.578 + 8.005x10⁻³TlnT - 3.754x10⁻⁶T² - 121.450T⁻¹ - 91.926x10⁻³T
368.3-388.36 K: ΔHf° = 31.347 - 3.479x10⁻³T + 0.262x10⁻⁶T² + 68.300T⁻¹
ΔGf° = 31.347 + 3.479x10⁻³TlnT - 0.262x10⁻⁶T² + 34.150T⁻¹ - 61.560x10⁻³T
388.36-432.02 K: ΔHf° = -0.969 + 86.001x10⁻³T - 86.302x10⁻⁶T² + 3872.700T⁻¹
ΔGf° = -0.969 - 86.001x10⁻³TlnT + 86.302x10⁻⁶T² + 1936.350T⁻¹ + 508.897x10⁻³T
432.02-717.824 K: ΔHf° = -19.927 + 78.189x10⁻³T - 46.678x10⁻⁶T² + 10325.700T⁻¹
ΔGf° = -19.927 - 78.189x10⁻³TlnT + 46.678x10⁻⁶T² + 5162.850T⁻¹ + 505.202x10⁻³T

$S_3(g)$
Sulfur (ideal triatomic gas)
[Formation: $3S(c,l) = S_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	11.493	65.275	65.275	0	34.272	21.663	-15.879
300	11.514	65.346	65.276	.021	34.263	21.585	-15.724
368.3	12.088	67.776	65.521	.831	33.921	18.733	-11.116
368.3	12.088	67.776	65.521	.831	33.633	18.733	-11.116
388.36	12.256	68.422	65.654	1.075	33.520	17.926	-10.088
388.36	12.256	68.422	65.654	1.075	32.281	17.926	-10.088
400	12.354	68.785	65.740	1.218	32.160	17.497	-9.560
432.02	12.510	69.742	66.002	1.616	31.769	16.336	-8.264
500	12.840	71.599	66.639	2.480	30.611	14.007	-6.122
600	13.137	73.968	67.668	3.780	29.340	10.811	-3.938
700	13.327	76.008	68.717	5.104	28.264	7.810	-2.438
717.824	13.350	76.343	68.902	5.342	28.091	7.293	-2.220

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-3000 K: $C_p^\circ = 13.561 + 0.170 \times 10^{-3}T - 1.883 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 13.561 \times 10^{-3}T + 0.085 \times 10^{-6}T^2 + 1.883 \times 10^{-2}T^{-1} - 4.682$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 38.009 - 10.961 \times 10^{-3}T + 5.236 \times 10^{-6}T^2 - 278.500T^{-1}$
 $\Delta G_f^\circ = 38.009 + 10.961 \times 10^{-3}T \ln T - 5.236 \times 10^{-6}T^2 - 139.250T^{-1} - 114.149 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = 34.663 - 4.172 \times 10^{-3}T - 0.002 \times 10^{-6}T^2 + 188.300T^{-1}$
 $\Delta G_f^\circ = 34.663 + 4.172 \times 10^{-3}T \ln T + 0.002 \times 10^{-6}T^2 + 94.150T^{-1} - 68.600 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = -13.812 + 130.048 \times 10^{-3}T - 129.848 \times 10^{-6}T^2 + 5894.900T^{-1}$
 $\Delta G_f^\circ = -13.812 - 130.048 \times 10^{-3}T \ln T + 129.848 \times 10^{-6}T^2 + 2947.450T^{-1} + 787.085 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = -42.248 + 118.330 \times 10^{-3}T - 70.412 \times 10^{-6}T^2 + 15574.400T^{-1}$
 $\Delta G_f^\circ = -42.248 - 118.330 \times 10^{-3}T \ln T + 70.412 \times 10^{-6}T^2 + 7787.200T^{-1} + 781.543 \times 10^{-3}T$

$S_3(g)$
Sulfur (ideal triatomic gas)
[Reaction: $1.5S_2(g) = S_3(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15	11.493	65.275	65.275	0	-11.793	-6.878	5.042
300	11.514	65.346	65.276	.021	-11.793	-6.847	4.988
400	12.354	68.785	65.740	1.218	-11.793	-5.200	2.841
500	12.840	71.599	66.639	2.480	-11.771	-3.553	1.553
600	13.137	73.968	67.668	3.780	-11.743	-1.912	.696
700	13.327	76.008	68.717	5.104	-11.711	-.275	.086
800	13.457	77.797	69.742	6.444	-11.678	1.357	-.371
900	13.548	79.387	70.727	7.794	-11.647	2.983	-.724
1000	13.614	80.818	71.666	9.152	-11.620	4.608	-1.007
1100	13.664	82.118	72.557	10.517	-11.597	6.230	-1.238
1200	13.702	83.309	73.405	11.885	-11.583	7.850	-1.430
1300	13.733	84.407	74.209	13.257	-11.574	9.468	-1.592
1400	13.757	85.425	74.974	14.631	-11.576	11.088	-1.731
1500	13.776	86.375	75.703	16.008	-11.585	12.706	-1.851
1600	13.792	87.265	76.399	17.386	-11.603	14.325	-1.957
1700	13.806	88.101	77.062	18.766	-11.632	15.947	-2.050
1800	13.817	88.891	77.698	20.148	-11.666	17.571	-2.133
1900	13.826	89.638	78.307	21.529	-11.711	19.195	-2.208
2000	13.834	90.348	78.892	22.913	-11.763	20.824	-2.275
2100	13.841	91.023	79.453	24.296	-11.822	22.453	-2.337
2200	13.848	91.667	79.994	25.681	-11.888	24.087	-2.393
2300	13.853	92.283	80.515	27.066	-11.959	25.725	-2.444
2400	13.857	92.872	81.017	28.451	-12.038	27.365	-2.492
2500	13.862	93.438	81.503	29.837	-12.121	29.009	-2.536
2600	13.865	93.982	81.973	31.224	-12.209	30.654	-2.577
2700	13.869	94.505	82.427	32.610	-12.300	32.305	-2.615
2800	13.871	95.009	82.867	33.997	-12.396	33.962	-2.651
2900	13.874	95.496	83.294	35.385	-12.495	35.620	-2.684
3000	13.876	95.967	83.710	36.772	-12.598	37.276	-2.716

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

298.15-3000 K: $C_p^\circ = 13.561 + 0.170 \times 10^{-3}T - 1.883 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 13.561 \times 10^{-3}T + 0.085 \times 10^{-6}T^2 + 1.883 \times 10^{-2}T^{-1} - 4.682$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -12.358 + 1.046 \times 10^{-3}T - 0.395 \times 10^{-6}T^2 + 85.850T^{-1}$
 $\Delta G_r^\circ = -12.358 - 1.046 \times 10^{-3}T \ln T + 0.395 \times 10^{-6}T^2 + 42.925T^{-1} + 23.740 \times 10^{-3}T$
2000-3000 K: $\Delta H_r^\circ = -9.283 - 0.704 \times 10^{-3}T - 0.065 \times 10^{-6}T^2 - 1701.700T^{-1}$
 $\Delta G_r^\circ = -9.283 + 0.704 \times 10^{-3}T \ln T + 0.065 \times 10^{-6}T^2 - 850.850T^{-1} + 9.781 \times 10^{-3}T$

Source: Data from Pankratz (91).

$S_4(g)$
Sulfur (ideal tetratomic gas)
[Formation: $4S(c,1) = S_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	15.761	70.128	70.128	0	32.417	20.645	-15.133
300	15.796	70.226	70.129	.029	32.406	20.572	-14.987
368.3	16.772	73.581	70.464	1.148	31.989	17.921	-10.634
368.3	16.772	73.581	70.464	1.148	31.605	17.921	-10.634
388.36	17.059	74.479	70.649	1.487	31.468	17.182	-9.669
388.36	17.059	74.479	70.649	1.487	29.816	17.182	-9.669
400	17.225	74.985	70.768	1.687	29.664	16.804	-9.181
432.02	17.489	76.322	71.130	2.243	29.168	15.792	-7.989
500	18.050	78.925	72.017	3.454	27.683	13.814	-6.038
600	18.553	82.264	73.454	5.286	26.087	11.197	-4.079
700	18.877	85.150	74.923	7.159	24.760	8.824	-2.755
717.824	18.916	85.625	75.183	7.496	24.549	8.423	-2.564

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-3000 K: $C_p^\circ = 19.279 + 0.288 \times 10^{-3}T - 3.204 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 19.279 \times 10^{-3}T + 0.144 \times 10^{-6}T^2 + 3.204 \times 10^{-2}T^{-1} - 6.835$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 36.807 - 13.417 \times 10^{-3}T + 7.012 \times 10^{-6}T^2 - 302.000T^{-1}$
 $\Delta G_f^\circ = 36.807 + 13.417 \times 10^{-3}T \ln T - 7.012 \times 10^{-6}T^2 - 151.000T^{-1} - 126.863 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = 32.346 - 4.365 \times 10^{-3}T + 0.028 \times 10^{-6}T^2 + 320.400T^{-1}$
 $\Delta G_f^\circ = 32.346 + 4.365 \times 10^{-3}T \ln T - 0.028 \times 10^{-6}T^2 + 160.200T^{-1} - 66.131 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = -32.287 + 174.595 \times 10^{-3}T - 173.100 \times 10^{-6}T^2 + 7929.200T^{-1}$
 $\Delta G_f^\circ = -32.287 - 174.595 \times 10^{-3}T \ln T + 173.100 \times 10^{-6}T^2 + 3964.600T^{-1} + 1074.782 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = -70.202 + 158.971 \times 10^{-3}T - 93.852 \times 10^{-6}T^2 + 20835.200T^{-1}$
 $\Delta G_f^\circ = -70.202 - 158.971 \times 10^{-3}T \ln T + 93.852 \times 10^{-6}T^2 + 10417.600T^{-1} + 1067.392 \times 10^{-3}T$

$S_4(g)$
Sulfur (ideal tetratomic gas)
[Reaction: $2S_2(g) = S_4(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15	15.761	70.128	70.128	0	-29.003	-17.410	12.762
300	15.796	70.226	70.129	.029	-29.002	-17.337	12.630
400	17.225	74.985	70.768	1.687	-28.940	-13.458	7.353
500	18.050	78.925	72.017	3.454	-28.827	-9.598	4.195
600	18.553	82.264	73.454	5.286	-28.691	-5.766	2.100
700	18.877	85.150	74.923	7.159	-28.540	-1.957	.611
800	19.097	87.686	76.363	9.058	-28.383	1.831	-.500
900	19.253	89.945	77.749	10.976	-28.225	5.596	-1.359
1000	19.366	91.980	79.072	12.908	-28.067	9.347	-2.043
1100	19.451	93.829	80.330	14.849	-27.916	13.082	-2.599
1200	19.517	95.525	81.528	16.797	-27.772	16.802	-3.060
1300	19.568	97.089	82.665	18.751	-27.636	20.509	-3.448
1400	19.609	98.541	83.748	20.710	-27.511	24.209	-3.779
1500	19.642	99.895	84.780	22.673	-27.396	27.898	-4.065
1600	19.670	101.163	85.764	24.639	-27.292	31.583	-4.314
1700	19.693	102.357	86.706	26.607	-27.202	35.258	-4.533
1800	19.712	103.483	87.607	28.577	-27.120	38.931	-4.727
1900	19.728	104.549	88.471	30.549	-27.050	42.598	-4.900
2000	19.742	105.561	89.299	32.523	-26.990	46.264	-5.055
2100	19.754	106.525	90.098	34.497	-26.940	49.922	-5.195
2200	19.764	107.444	90.865	36.473	-26.898	53.582	-5.323
2300	19.773	108.323	91.606	38.450	-26.863	57.241	-5.439
2400	19.781	109.164	92.319	40.428	-26.837	60.897	-5.545
2500	19.789	109.972	93.010	42.406	-26.817	64.553	-5.643
2600	19.795	110.748	93.676	44.386	-26.803	68.206	-5.733
2700	19.800	111.495	94.323	46.365	-26.794	71.861	-5.817
2800	19.805	112.216	94.950	48.346	-26.791	75.515	-5.894
2900	19.810	112.911	95.557	50.326	-26.793	79.170	-5.966
3000	19.814	113.582	96.146	52.308	-26.797	82.823	-6.034

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

298.15-3000 K: $C_p^\circ = 19.279 + 0.288 \times 10^{-3}T - 3.204 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 19.279 \times 10^{-3}T + 0.144 \times 10^{-6}T^2 + 3.204 \times 10^{-2}T^{-1} - 6.835$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -30.348 + 2.593 \times 10^{-3}T - 0.496 \times 10^{-6}T^2 + 183.800T^{-1}$
 $\Delta G_r^\circ = -30.348 - 2.593 \times 10^{-3}T \ln T + 0.496 \times 10^{-6}T^2 + 91.900T^{-1} + 56.989 \times 10^{-3}T$
2000-3000 K: $\Delta H_r^\circ = -26.249 + 0.259 \times 10^{-3}T - 0.056 \times 10^{-6}T^2 - 2199.600T^{-1}$
 $\Delta G_r^\circ = -26.249 - 0.259 \times 10^{-3}T \ln T + 0.056 \times 10^{-6}T^2 - 1099.800T^{-1} + 38.376 \times 10^{-3}T$

Source: Data from Pankratz (91).

$S_8(g)$
Sulfur (ideal pentatomic gas)
[Formation: $5S(c,l) = S_8(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	21.331	80.629	80.629	0	29.704	17.085	-12.524
300	21.373	80.761	80.629	.040	29.694	17.008	-12.390
368.3	22.508	85.283	81.082	1.547	29.281	14.161	-8.403
368.3	22.508	85.283	81.082	1.547	28.801	14.161	-8.403
388.36	22.842	86.486	81.331	2.002	28.661	13.371	-7.524
388.36	22.842	86.486	81.331	2.002	26.596	13.371	-7.524
400	23.035	87.163	81.491	2.269	26.423	12.976	-7.090
432.02	23.325	88.948	81.978	3.011	25.850	11.918	-6.029
500	23.941	92.410	83.166	4.622	24.091	9.878	-4.318
600	24.478	96.826	85.084	7.045	22.229	7.219	-2.630
700	24.818	100.627	87.040	9.511	20.695	4.842	-1.512
717.824	24.859	101.251	87.385	9.954	20.453	4.444	-1.353

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: $C_p^\circ = 25.297 + 0.306 \times 10^{-3}T - 3.607 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 25.297 \times 10^{-3}T + 0.153 \times 10^{-6}T^2 + 3.607 \times 10^{-2}T^{-1} - 8.766$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 34.970 - 15.573 \times 10^{-3}T + 8.738 \times 10^{-6}T^2 - 417.300T^{-1}$
 $\Delta G_f^\circ = 34.970 + 15.573 \times 10^{-3}T \ln T - 8.738 \times 10^{-6}T^2 - 208.650T^{-1} - 143.762 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = 29.394 - 4.258 \times 10^{-3}T + 0.008 \times 10^{-6}T^2 + 360.700T^{-1}$
 $\Delta G_f^\circ = 29.394 + 4.258 \times 10^{-3}T \ln T - 0.008 \times 10^{-6}T^2 + 180.350T^{-1} - 67.848 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = -51.397 + 219.442 \times 10^{-3}T - 216.402 \times 10^{-6}T^2 + 9871.700T^{-1}$
 $\Delta G_f^\circ = -51.397 - 219.442 \times 10^{-3}T \ln T + 216.402 \times 10^{-6}T^2 + 4935.850T^{-1} + 1358.294 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = -98.791 + 199.912 \times 10^{-3}T - 117.342 \times 10^{-6}T^2 + 26004.200T^{-1}$
 $\Delta G_f^\circ = -98.791 - 199.912 \times 10^{-3}T \ln T + 117.342 \times 10^{-6}T^2 + 13002.100T^{-1} + 1349.057 \times 10^{-3}T$

$S_5(g)$
Sulfur (ideal pentatomic gas)
[Reaction: $2.5S_2(g) = S_5(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15	21.331	80.629	80.629	0	-47.071	-30.483	22.344
300	21.373	80.761	80.629	.040	-47.066	-30.378	22.130
400	23.035	87.163	81.491	2.269	-46.832	-24.852	13.578
500	23.941	92.410	83.166	4.622	-46.546	-19.388	8.474
600	24.478	96.826	85.084	7.045	-46.243	-13.985	5.094
700	24.818	100.627	87.040	9.511	-45.930	-8.634	2.696
800	25.046	103.957	88.951	12.005	-45.614	-3.325	.908
900	25.206	106.917	90.786	14.518	-45.300	1.939	-.471
1000	25.322	109.579	92.534	17.045	-44.991	7.172	-1.568
1100	25.409	111.996	94.194	19.582	-44.691	12.375	-2.459
1200	25.475	114.210	95.772	22.126	-44.402	17.550	-3.196
1300	25.528	116.251	97.269	24.676	-44.125	22.700	-3.816
1400	25.569	118.145	98.694	27.231	-43.862	27.831	-4.345
1500	25.603	119.910	100.050	29.790	-43.613	32.943	-4.800
1600	25.630	121.563	101.344	32.351	-43.380	38.039	-5.196
1700	25.653	123.118	102.579	34.916	-43.162	43.120	-5.543
1800	25.673	124.585	103.762	37.482	-42.957	48.191	-5.851
1900	25.689	125.973	104.894	40.050	-42.766	53.250	-6.125
2000	25.703	127.291	105.981	42.620	-42.589	58.299	-6.371
2100	25.715	128.546	107.026	45.191	-42.422	63.337	-6.591
2200	25.725	129.742	108.032	47.763	-42.268	68.371	-6.792
2300	25.735	130.886	109.001	50.336	-42.123	73.398	-6.974
2400	25.743	131.981	109.936	52.909	-41.990	78.416	-7.141
2500	25.750	133.032	110.838	55.484	-41.862	83.433	-7.294
2600	25.756	134.042	111.712	58.059	-41.745	88.439	-7.434
2700	25.762	135.015	112.558	60.635	-41.631	93.443	-7.564
2800	25.767	135.951	113.375	63.212	-41.527	98.450	-7.684
2900	25.771	136.856	114.170	65.789	-41.427	103.447	-7.796
3000	25.775	137.729	114.940	68.366	-41.333	108.438	-7.900

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

298.15-2000 K: $C_p^\circ = 25.297 + 0.306 \times 10^{-3}T - 3.607 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 25.297 \times 10^{-3}T + 0.153 \times 10^{-6}T^2 + 3.607 \times 10^2 T^{-1} - 8.766$
 2000-3000 K: $C_p^\circ = 26.003 - 0.050 \times 10^{-3}T - 7.986 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 26.003 \times 10^{-3}T - 0.025 \times 10^{-6}T^2 + 7.986 \times 10^2 T^{-1} - 9.685$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -48.974 + 4.439 \times 10^{-3}T - 0.647 \times 10^{-6}T^2 + 189.950T^{-1}$
 $\Delta G_r^\circ = -48.974 - 4.439 \times 10^{-3}T \ln T + 0.647 \times 10^{-6}T^2 + 94.975T^{-1} + 86.053 \times 10^{-3}T$
 2000-3000 K: $\Delta H_r^\circ = -44.769 + 2.228 \times 10^{-3}T - 0.275 \times 10^{-6}T^2 - 2351.400T^{-1}$
 $\Delta G_r^\circ = -44.769 - 2.228 \times 10^{-3}T \ln T + 0.275 \times 10^{-6}T^2 - 1175.700T^{-1} + 68.202 \times 10^{-3}T$

Source: Data from Pankratz (91).

$S_6(g)$
Sulfur (ideal hexatomic gas)
[Formation: $6S(c,l) = S_6(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	26.901	84.555	84.555	0	24.004	12.499	-9.162
300	26.951	84.721	84.555	.050	23.994	12.429	-9.054
368.3	28.245	90.409	85.125	1.946	23.586	9.835	-5.836
368.3	28.245	90.409	85.125	1.946	23.010	9.835	-5.836
388.36	28.625	91.917	85.438	2.517	22.867	9.127	-5.136
388.36	28.625	91.917	85.438	2.517	20.389	9.127	-5.136
400	28.846	92.766	85.638	2.851	20.195	8.790	-4.803
432.02	29.162	95.000	86.251	3.780	19.546	7.899	-3.996
500	29.834	99.319	87.741	5.789	17.511	6.242	-2.729
600	30.403	104.813	90.140	8.804	15.384	4.199	-1.530
700	30.759	109.529	92.582	11.863	13.643	2.476	-.773
717.824	30.801	110.303	93.012	12.411	13.369	2.198	-.669

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $C_p^\circ = 31.351 + 0.262 \times 10^{-3}T - 4.027 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 31.351 \times 10^{-3}T + 0.131 \times 10^{-6}T^2 + 4.027 \times 10^{-2}T^{-1} - 10.710$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 30.132 - 17.693 \times 10^{-3}T + 10.433 \times 10^{-6}T^2 - 530.900T^{-1}$
 $\Delta G_f^\circ = 30.132 + 17.693 \times 10^{-3}T \ln T - 10.433 \times 10^{-6}T^2 - 265.450T^{-1} - 153.855 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = 23.442 - 4.115 \times 10^{-3}T - 0.043 \times 10^{-6}T^2 + 402.700T^{-1}$
 $\Delta G_f^\circ = 23.442 + 4.115 \times 10^{-3}T \ln T + 0.043 \times 10^{-6}T^2 + 201.350T^{-1} - 62.757 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = -73.508 + 264.325 \times 10^{-3}T - 259.735 \times 10^{-6}T^2 + 11815.900T^{-1}$
 $\Delta G_f^\circ = -73.508 - 264.325 \times 10^{-3}T \ln T + 259.735 \times 10^{-6}T^2 + 5907.950T^{-1} + 1648.613 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = -130.380 + 240.889 \times 10^{-3}T - 140.863 \times 10^{-6}T^2 + 31174.900T^{-1}$
 $\Delta G_f^\circ = -130.380 - 240.889 \times 10^{-3}T \ln T + 140.863 \times 10^{-6}T^2 + 15587.450T^{-1} + 1637.528 \times 10^{-3}T$

$S_6(g)$
Sulfur (ideal hexatomic gas)
[Reaction: $3S_2(g) = S_6(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15	26.901	84.555	84.555	0	-68.126	-44.583	32.680
300	26.951	84.721	84.555	.050	-68.118	-44.435	32.370
400	28.846	92.766	85.638	2.851	-67.711	-36.603	19.999
500	29.834	99.319	87.741	5.789	-67.254	-28.877	12.622
600	30.403	104.813	90.140	8.804	-66.783	-21.246	7.739
700	30.759	109.529	92.582	11.863	-66.307	-13.695	4.276
800	30.995	113.652	94.962	14.952	-65.831	-6.208	1.696
900	31.159	117.313	97.246	18.060	-65.363	1.213	-.294
1000	31.278	120.603	99.421	21.182	-64.902	8.586	-1.876
1100	31.366	123.588	101.484	24.314	-64.455	15.913	-3.162
1200	31.434	126.321	103.442	27.455	-64.020	23.201	-4.225
1300	31.487	128.839	105.300	30.601	-63.601	30.450	-5.119
1400	31.529	131.174	107.066	33.751	-63.202	37.671	-5.881
1500	31.563	133.350	108.746	36.906	-62.819	44.861	-6.536
1600	31.591	135.388	110.348	40.064	-62.454	52.029	-7.107
1700	31.614	137.304	111.878	43.224	-62.111	59.172	-7.607
1800	31.633	139.112	113.341	46.387	-61.780	66.299	-8.050
1900	31.650	140.822	114.743	49.551	-61.469	73.406	-8.444
2000	31.664	142.446	116.088	52.717	-61.174	80.498	-8.796
2100	31.676	143.991	117.380	55.883	-60.894	87.572	-9.114
2200	31.687	145.465	118.623	59.052	-60.626	94.637	-9.401
2300	31.696	146.874	119.821	62.221	-60.370	101.690	-9.663
2400	31.704	148.223	120.977	65.391	-60.128	108.729	-9.901
2500	31.711	149.517	122.093	68.561	-59.895	115.763	-10.120
2600	31.718	150.761	123.171	71.733	-59.672	122.780	-10.320
2700	31.723	151.958	124.215	74.905	-59.455	129.796	-10.506
2800	31.728	153.112	125.227	78.077	-59.250	136.803	-10.678
2900	31.733	154.226	126.208	81.251	-59.049	143.803	-10.837
3000	31.737	155.301	127.160	84.424	-58.855	150.791	-10.985

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

298.15-2000 K: $C_p^\circ = 31.351 + 0.262 \times 10^{-3}T - 4.027 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 31.351 \times 10^{-3}T + 0.131 \times 10^{-6}T^2 + 4.027 \times 10^2 T^{-1} - 10.710$
 2000-3000 K: $C_p^\circ = 29.750 + 0.600 \times 10^{-3}T + 28.557 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 29.750 \times 10^{-3}T + 0.300 \times 10^{-6}T^2 - 28.557 \times 10^2 T^{-1} - 6.555$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -70.601 + 6.322 \times 10^{-3}T - 0.829 \times 10^{-6}T^2 + 197.800T^{-1}$
 $\Delta G_r^\circ = -70.601 - 6.322 \times 10^{-3}T \ln T + 0.829 \times 10^{-6}T^2 + 98.900T^{-1} + 121.923 \times 10^{-3}T$
 2000-3000 K: $\Delta H_r^\circ = -60.296 + 1.220 \times 10^{-3}T \ln T - 6635.700T^{-1}$
 $\Delta G_r^\circ = -60.296 - 1.220 \times 10^{-3}T \ln T - 3317.850T^{-1} + 80.503 \times 10^{-3}T$

Source: Data from Pankratz (91).

$S_7(g)$
Sulfur (ideal heptatomic gas)
[Formation: $7S(c,1) = S_7(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	31.990	95.508	95.508	0	25.669	13.182	-9.663
300	32.049	95.706	95.509	.059	25.658	13.106	-9.547
368.3	33.570	102.467	96.188	2.313	25.224	10.290	-6.106
368.3	33.570	102.467	96.188	2.313	24.552	10.290	-6.106
388.36	34.017	104.260	96.559	2.991	24.397	9.523	-5.359
388.36	34.017	104.260	96.559	2.991	21.506	9.523	-5.359
400	34.276	105.268	96.798	3.388	21.287	9.165	-5.007
432.02	34.649	107.922	97.525	4.491	20.549	8.219	-4.158
500	35.440	113.054	99.294	6.880	18.220	6.483	-2.833
600	36.112	119.580	102.147	10.460	15.801	4.373	-1.593
700	36.532	125.181	105.047	14.094	13.835	2.629	-.821
717.824	36.582	126.100	105.558	14.745	13.527	2.351	-.716

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $C_p^\circ = 37.220 + 0.316 \times 10^{-3}T - 4.734 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 37.220 \times 10^{-3}T + 0.158 \times 10^{-6}T^2 + 4.734 \times 10^{-2}T^{-1} - 12.699$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 32.614 - 19.998 \times 10^{-3}T + 12.177 \times 10^{-6}T^2 - 615.800T^{-1}$
 $\Delta G_f^\circ = 32.614 + 19.998 \times 10^{-3}T \ln T - 12.177 \times 10^{-6}T^2 - 307.900T^{-1} - 172.022 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = 24.809 - 4.157 \times 10^{-3}T - 0.045 \times 10^{-6}T^2 + 473.400T^{-1}$
 $\Delta G_f^\circ = 24.809 + 4.157 \times 10^{-3}T \ln T + 0.045 \times 10^{-6}T^2 + 236.700T^{-1} - 65.741 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = -88.300 + 309.023 \times 10^{-3}T - 303.019 \times 10^{-6}T^2 + 13788.800T^{-1}$
 $\Delta G_f^\circ = -88.300 - 309.023 \times 10^{-3}T \ln T + 303.019 \times 10^{-6}T^2 + 6894.400T^{-1} + 1930.857 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = -154.650 + 281.681 \times 10^{-3}T - 164.335 \times 10^{-6}T^2 + 36374.300T^{-1}$
 $\Delta G_f^\circ = -154.650 - 281.681 \times 10^{-3}T \ln T + 164.335 \times 10^{-6}T^2 + 18187.150T^{-1} + 1917.925 \times 10^{-3}T$

$S_7(g)$
Sulfur (ideal heptatomic gas)
[Reaction: $3.5S_2(g) = S_7(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15	31.990	95.508	95.508	0	-81.816	-53.413	39.153
300	32.049	95.706	95.509	.059	-81.806	-53.235	38.781
400	34.276	105.268	96.798	3.388	-81.270	-43.794	23.928
500	35.440	113.054	99.294	6.880	-80.673	-34.490	15.075
600	36.112	119.580	102.147	10.460	-80.061	-25.313	9.220
700	36.532	125.181	105.047	14.094	-79.440	-16.237	5.069
800	36.811	130.078	107.876	17.762	-78.821	-7.247	1.980
900	37.005	134.426	110.589	21.453	-78.209	1.657	-.402
1000	37.145	138.332	113.171	25.161	-77.606	10.501	-2.295
1100	37.249	141.878	115.623	28.881	-77.018	19.283	-3.831
1200	37.329	145.122	117.947	32.610	-76.446	28.014	-5.102
1300	37.392	148.113	120.155	36.346	-75.892	36.693	-6.169
1400	37.441	150.886	122.252	40.088	-75.359	45.336	-7.077
1500	37.482	153.470	124.247	43.834	-74.847	53.937	-7.859
1600	37.515	155.890	126.150	47.584	-74.356	62.508	-8.538
1700	37.542	158.166	127.968	51.337	-73.889	71.045	-9.133
1800	37.565	160.312	129.705	55.093	-73.437	79.562	-9.660
1900	37.585	162.344	131.370	58.850	-73.009	88.047	-10.128
2000	37.602	164.272	132.967	62.610	-72.599	96.516	-10.547
2100	37.616	166.107	134.502	66.370	-72.205	104.958	-10.923
2200	37.628	167.857	135.979	70.132	-71.828	113.387	-11.264
2300	37.639	169.530	137.401	73.896	-71.463	121.801	-11.574
2400	37.649	171.132	138.774	77.660	-71.114	130.193	-11.856
2500	37.657	172.669	140.099	81.426	-70.775	138.577	-12.114
2600	37.665	174.146	141.380	85.192	-70.450	146.940	-12.351
2700	37.671	175.568	142.621	88.958	-70.131	155.296	-12.570
2800	37.677	176.938	143.822	92.726	-69.825	163.644	-12.773
2900	37.683	178.260	144.986	96.494	-69.525	171.980	-12.961
3000	37.688	179.538	146.117	100.262	-69.233	180.294	-13.134

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

298.15-2000 K: $C_p^\circ = 37.220 + 0.316 \times 10^{-3}T - 4.734 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 37.220 \times 10^{-3}T + 0.158 \times 10^{-6}T^2 + 4.734 \times 10^{-2}T^{-1} - 12.699$
 2000-3000 K: $C_p^\circ = 37.582 + 0.050 \times 10^{-3}T - 3.218 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 37.582 \times 10^{-3}T + 0.025 \times 10^{-6}T^2 + 3.218 \times 10^{-2}T^{-1} - 12.815$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -84.908 + 8.019 \times 10^{-3}T - 0.962 \times 10^{-6}T^2 + 234.350T^{-1}$
 $\Delta G_r^\circ = -84.908 - 8.019 \times 10^{-3}T \ln T + 0.962 \times 10^{-6}T^2 + 117.175T^{-1} + 149.719 \times 10^{-3}T$
 2000-3000 K: $\Delta H_r^\circ = -77.849 + 4.297 \times 10^{-3}T - 0.325 \times 10^{-6}T^2 - 4088.200T^{-1}$
 $\Delta G_r^\circ = -77.849 - 4.297 \times 10^{-3}T \ln T + 0.325 \times 10^{-6}T^2 - 2044.100T^{-1} + 119.710 \times 10^{-3}T$

Source: Data from Pankratz (91).

$S_8(g)$
Sulfur (ideal octatomic gas)
[Formation: $8S(c,l) = S_8(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	37.186	101.741	101.741	0	23.881	11.820	-8.664
300	37.251	101.971	101.741	.069	23.870	11.747	-8.557
368.3	38.965	109.823	102.529	2.686	23.415	9.030	-5.358
368.3	38.965	109.823	102.529	2.686	22.647	9.030	-5.358
388.36	39.469	111.903	102.961	3.473	22.482	8.299	-4.670
388.36	39.469	111.903	102.961	3.473	19.178	8.299	-4.670
400	39.761	113.073	103.238	3.934	18.935	7.975	-4.357
432.02	40.183	116.151	104.082	5.214	18.111	7.124	-3.604
500	41.080	122.101	106.137	7.982	15.487	5.625	-2.458
600	41.844	129.664	109.444	12.132	12.781	3.920	-1.428
700	42.322	136.153	112.807	16.342	10.591	2.621	-.818
717.824	42.378	137.218	113.400	17.097	10.250	2.427	-.739

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $C_p^\circ = 43.137 + 0.332 \times 10^{-3}T - 5.378 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 43.137 \times 10^{-3}T + 0.166 \times 10^{-6}T^2 + 5.378 \times 10^{-2}T^{-1} - 14.680$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 31.652 - 22.255 \times 10^{-3}T + 13.902 \times 10^{-6}T^2 - 707.000T^{-1}$
 $\Delta G_f^\circ = 31.652 + 22.255 \times 10^{-3}T \ln T - 13.902 \times 10^{-6}T^2 - 353.500T^{-1} - 185.195 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = 22.731 - 4.151 \times 10^{-3}T - 0.066 \times 10^{-6}T^2 + 537.800T^{-1}$
 $\Delta G_f^\circ = 22.731 + 4.151 \times 10^{-3}T \ln T + 0.066 \times 10^{-6}T^2 + 268.900T^{-1} - 63.731 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = -106.536 + 353.769 \times 10^{-3}T - 346.322 \times 10^{-6}T^2 + 15755.400T^{-1}$
 $\Delta G_f^\circ = -106.536 - 353.769 \times 10^{-3}T \ln T + 346.322 \times 10^{-6}T^2 + 7877.700T^{-1} + 2218.095 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = -182.365 + 322.521 \times 10^{-3}T - 187.826 \times 10^{-6}T^2 + 41567.400T^{-1}$
 $\Delta G_f^\circ = -182.365 - 322.521 \times 10^{-3}T \ln T + 187.826 \times 10^{-6}T^2 + 20783.700T^{-1} + 2203.315 \times 10^{-3}T$

$S_8(g)$
Sulfur (ideal octatomic gas)
[Reaction: $4S_2(g) = S_8(g)$]

T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15	37.186	101.741	101.741	0	-98.959	-64.289	47.125
300	37.251	101.971	101.741	.069	-98.946	-64.071	46.675
400	39.761	113.073	103.238	3.934	-98.273	-52.550	28.712
500	41.080	122.101	106.137	7.982	-97.533	-41.201	18.009
600	41.844	129.664	109.444	12.132	-96.775	-30.007	10.930
700	42.322	136.153	112.807	16.342	-96.009	-18.940	5.913
800	42.639	141.826	116.087	20.591	-95.244	-7.978	2.180
900	42.860	146.862	119.233	24.866	-94.489	2.878	-.699
1000	43.020	151.386	122.225	29.161	-93.742	13.660	-2.985
1100	43.139	155.492	125.066	33.469	-93.014	24.365	-4.841
1200	43.230	159.250	127.760	37.788	-92.303	35.005	-6.375
1300	43.302	162.713	130.318	42.114	-91.613	45.582	-7.663
1400	43.359	165.924	132.748	46.447	-90.948	56.114	-8.760
1500	43.404	168.918	135.061	50.786	-90.305	66.592	-9.702
1600	43.442	171.720	137.265	55.128	-89.687	77.033	-10.522
1700	43.474	174.355	139.370	59.474	-89.097	87.433	-11.240
1800	43.500	176.840	141.383	63.822	-88.525	97.804	-11.875
1900	43.522	179.193	143.312	68.174	-87.977	108.139	-12.439
2000	43.541	181.426	145.162	72.527	-87.452	118.448	-12.943
2100	43.557	183.550	146.940	76.882	-86.945	128.729	-13.397
2200	43.572	185.577	148.651	81.238	-86.457	138.988	-13.807
2300	43.584	187.514	150.298	85.596	-85.983	149.229	-14.180
2400	43.595	189.369	151.888	89.955	-85.528	159.442	-14.519
2500	43.605	191.149	153.423	94.315	-85.084	169.644	-14.830
2600	43.613	192.859	154.907	98.676	-84.655	179.820	-15.115
2700	43.621	194.506	156.344	103.038	-84.233	189.984	-15.378
2800	43.628	196.092	157.735	107.400	-83.827	200.138	-15.621
2900	43.634	197.623	159.084	111.763	-83.428	210.275	-15.847
3000	43.639	199.103	160.394	116.127	-83.036	220.387	-16.055

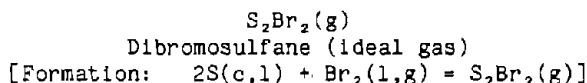
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 43.137 + 0.332 \times 10^{-3}T - 5.378 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 43.137 \times 10^{-3}T + 0.166 \times 10^{-6}T^2 + 5.378 \times 10^{-2}T^{-1} - 14.680$
 2000-3000 K: $C_p^\circ = 43.703 + 0.004 \times 10^{-3}T - 6.801 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 43.703 \times 10^{-3}T + 0.002 \times 10^{-6}T^2 + 6.801 \times 10^{-2}T^{-1} - 15.227$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -102.659 + 9.765 \times 10^{-3}T - 1.114 \times 10^{-6}T^2 + 264.600T^{-1}$
 $\Delta G_r^\circ = -102.659 - 9.765 \times 10^{-3}T \ln T + 1.114 \times 10^{-6}T^2 + 132.300T^{-1} + 182.509 \times 10^{-3}T$
 2000-3000 K: $\Delta H_r^\circ = -95.007 + 5.663 \times 10^{-3}T - 0.398 \times 10^{-6}T^2 - 4359.900T^{-1}$
 $\Delta G_r^\circ = -95.007 - 5.663 \times 10^{-3}T \ln T + 0.398 \times 10^{-6}T^2 - 2179.950T^{-1} + 149.514 \times 10^{-3}T$

Source: Data from Pankratz (91).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHf°	ΔGf°	
298.15*	17.980	83.750	83.750	0	7.400	-2.155	1.580
300	18.010	83.860	83.750	.033	7.380	-2.214	1.613
332.6	18.264	85.731	83.854	.624	7.023	-3.238	2.128
332.6	18.264	85.731	83.854	.624	-.042	-3.238	2.128
368.3	18.543	87.619	84.126	1.286	-.099	-3.581	2.125
368.3	18.543	87.619	84.126	1.286	-.291	-3.581	2.125
388.36	18.699	88.606	84.333	1.660	-.331	-3.757	2.114
388.36	18.699	88.606	84.333	1.660	-1.157	-3.757	2.114
400	18.790	89.160	84.465	1.878	-1.217	-3.835	2.095
432.02	18.915	90.612	84.867	2.482	-1.421	-4.038	2.043
500	19.180	93.400	85.844	3.778	-2.073	-4.394	1.921
600	19.420	96.920	87.405	5.709	-2.744	-4.791	1.745
700	19.600	99.930	88.986	7.661	-3.285	-5.090	1.589
717.824	19.623	100.423	89.264	8.010	-3.369	-5.133	1.563

*Enthalpy of formation at 298 K estimated.

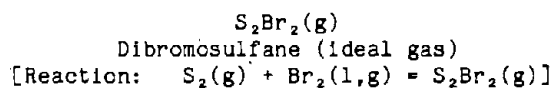
Phase changes: 332.6 K, boiling point of Br_2 ; $\Delta\text{H}^\circ = 7.065$ kcal/mol.
 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta\text{H}^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta\text{H}^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta\text{H}^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-1000 K: $\text{Cp}^\circ = 19.445 + 0.648 \times 10^{-3}T - 1.469 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 19.445 \times 10^{-3}T + 0.324 \times 10^{-6}T^2 + 1.469 \times 10^{-2}T^{-1} - 6.319$

Formation equations (kcal/mol):

298.15-332.6 K: $\Delta\text{Hf}^\circ = 12.079 - 14.994 \times 10^{-3}T + 3.858 \times 10^{-6}T^2 - 164.300T^{-1}$
 $\Delta\text{Gf}^\circ = 12.079 + 14.994 \times 10^{-3}T \ln T - 3.858 \times 10^{-6}T^2 - 82.150T^{-1} - 131.096 \times 10^{-3}T$
 332.6-368.3 K: $\Delta\text{Hf}^\circ = 2.078 - 5.833 \times 10^{-3}T + 3.703 \times 10^{-6}T^2 - 195.700T^{-1}$
 $\Delta\text{Gf}^\circ = 2.078 + 5.833 \times 10^{-3}T \ln T - 3.703 \times 10^{-6}T^2 - 97.850T^{-1} - 47.741 \times 10^{-3}T$
 368.3-388.36 K: $\Delta\text{Hf}^\circ = -0.152 - 1.307 \times 10^{-3}T + 0.211 \times 10^{-6}T^2 + 115.500T^{-1}$
 $\Delta\text{Gf}^\circ = -0.152 + 1.307 \times 10^{-3}T \ln T - 0.211 \times 10^{-6}T^2 + 57.750T^{-1} - 17.375 \times 10^{-3}T$
 388.36-432.02 K: $\Delta\text{Hf}^\circ = -32.469 + 88.173 \times 10^{-3}T - 86.353 \times 10^{-6}T^2 + 3919.900T^{-1}$
 $\Delta\text{Gf}^\circ = -32.469 - 88.173 \times 10^{-3}T \ln T + 86.353 \times 10^{-6}T^2 + 1959.950T^{-1} + 553.081 \times 10^{-3}T$
 432.02-717.824 K: $\Delta\text{Hf}^\circ = -51.426 + 80.361 \times 10^{-3}T - 46.729 \times 10^{-6}T^2 + 10372.900T^{-1}$
 $\Delta\text{Gf}^\circ = -51.426 - 80.361 \times 10^{-3}T \ln T + 46.729 \times 10^{-6}T^2 + 5186.450T^{-1} + 549.386 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/T$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHr°	ΔGr°	
298.15*	17.980	83.750	83.750	0	-23.310	-21.183	15.527
300	18.010	83.860	83.750	.033	-23.324	-21.168	15.421
332.6	18.264	85.731	83.854	.624	-23.576	-20.921	13.747
332.6	18.264	85.731	83.854	.624	-30.641	-20.921	13.747
400	18.790	89.160	84.465	1.878	-30.519	-18.966	10.363
500	19.180	93.400	85.844	3.778	-30.328	-16.101	7.037
600	19.420	96.920	87.405	5.709	-30.133	-13.273	4.835
700	19.600	99.930	88.986	7.661	-29.935	-10.480	3.272
800	19.730	102.560	90.525	9.628	-29.734	-7.716	2.108
900	19.850	104.890	91.993	11.607	-29.534	-4.977	1.208
1000	19.940	106.980	93.384	13.596	-29.332	-2.253	.492

*Enthalpy of formation at 298 K estimated.

Phase change: 332.6 K, boiling point of Br_2 ; $\Delta\text{H}^\circ = 7.065$ kcal/mol.

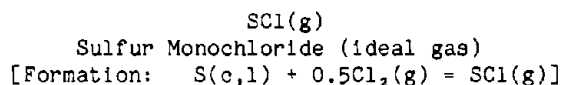
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $\text{Cp}^\circ = 19.445 + 0.648 \times 10^{-3}T - 1.469 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 19.445 \times 10^{-3}T + 0.324 \times 10^{-6}T^2 + 1.469 \times 10^{-2}T^{-1} - 6.319$

Reaction equations (kcal/mol):

298.15-332.6 K: $\Delta\text{Hr}^\circ = -21.499 - 6.989 \times 10^{-3}T + 0.104 \times 10^{-6}T^2 + 78.600T^{-1}$
 $\Delta\text{Gr}^\circ = -21.499 + 6.989 \times 10^{-3}T \ln T - 0.104 \times 10^{-6}T^2 + 39.300T^{-1} - 39.170 \times 10^{-3}T$
 332.6-1000 K: $\Delta\text{Hr}^\circ = -31.499 + 2.172 \times 10^{-3}T - 0.051 \times 10^{-6}T^2 + 47.200T^{-1}$
 $\Delta\text{Gr}^\circ = -31.499 - 2.172 \times 10^{-3}T \ln T + 0.051 \times 10^{-6}T^2 + 23.600T^{-1} + 44.185 \times 10^{-3}T$

Source: Data from Mills (80) who estimated enthalpy of formation at 298 K.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H _{2,98} °)/T	H°- H _{2,98} °	ΔHf°	ΔGf°	
298.15*	8.973	56.696	56.696	0	37.400	30.724	-22.521
300	8.977	56.751	56.696	.017	37.399	30.684	-22.353
368.3	9.061	58.605	56.883	.634	37.351	29.158	-17.302
368.3	9.061	58.605	56.883	.634	37.255	29.158	-17.302
388.36	9.086	59.086	56.985	.816	37.234	28.719	-16.161
388.36	9.086	59.086	56.985	.816	36.821	28.719	-16.161
400	9.100	59.355	57.050	.922	36.790	28.476	-15.558
432.02	9.105	60.056	57.247	1.213	36.682	27.814	-14.070
500	9.116	61.388	57.722	1.833	36.337	26.449	-11.561
600	9.108	63.050	58.477	2.744	35.957	24.508	-8.927
700	9.099	64.453	59.232	3.655	35.629	22.627	-7.064
717.824	9.098	64.682	59.364	3.817	35.575	22.297	-6.789

*Data estimated.

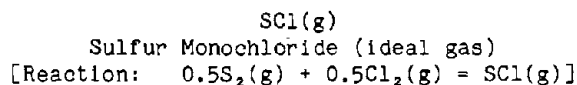
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 9.204 - 0.068x10⁻³T - 0.188x10⁻⁵T⁻²
H°- H_{2,98}° = 9.204x10⁻³T - 0.034x10⁻⁶T² + 0.188x10⁻²T⁻¹ - 2.804

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 38.836 - 3.383x10⁻³T + 1.639x10⁻⁶T² - 170.950T⁻¹
ΔGf° = 38.836 + 3.383x10⁻³TlnT - 1.639x10⁻⁶T² - 85.475T⁻¹ - 45.036x10⁻³T
368.3-388.36 K: ΔHf° = 37.721 - 1.120x10⁻³T - 0.107x10⁻⁶T² - 15.350T⁻¹
ΔGf° = 37.721 + 1.120x10⁻³TlnT + 0.107x10⁻⁶T² - 7.675T⁻¹ - 29.853x10⁻³T
388.36-432.02 K: ΔHf° = 21.563 + 43.619x10⁻³T - 43.389x10⁻⁶T² + 1886.850T⁻¹
ΔGf° = 21.563 - 43.619x10⁻³TlnT + 43.389x10⁻⁶T² + 943.425T⁻¹ + 255.376x10⁻³T
432.02-717.824 K: ΔHf° = 12.084 + 39.714x10⁻³T - 23.577x10⁻⁶T² + 5113.350T⁻¹
ΔGf° = 12.084 - 39.714x10⁻³TlnT + 23.577x10⁻⁶T² + 2556.675T⁻¹ + 253.528x10⁻³T



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.

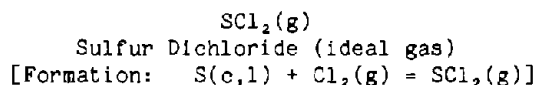
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 9.204 - 0.068 \times 10^{-3}T - 0.188 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 9.204 \times 10^{-3}T - 0.034 \times 10^{-6}T^2 + 0.188 \times 10^{-2}T^{-1} - 2.804$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = 22.048 + 0.619 \times 10^{-3}T - 0.238 \times 10^{-6}T^2 - 49.500T^{-1}$
 $\Delta G_r^\circ = 22.048 - 0.619 \times 10^{-3}T \ln T + 0.238 \times 10^{-6}T^2 - 24.750T^{-1} + 0.927 \times 10^{-3}T$

Source: Data from Pankratz (92).



T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	12.164	67.285	67.285	0	-4.200	-6.088	4.463
300	12.180	67.360	67.285	.023	-4.202	-6.100	4.443
368.3	12.618	69.912	67.542	.873	-4.300	-6.522	3.870
368.3	12.618	69.912	67.542	.873	-4.396	-6.522	3.870
388.36	12.746	70.584	67.682	1.127	-4.429	-6.637	3.735
388.36	12.746	70.584	67.682	1.127	-4.842	-6.637	3.735
400	12.821	70.962	67.772	1.276	-4.879	-6.690	3.655
432.02	12.934	71.954	68.046	1.688	-5.001	-6.831	3.456
500	13.173	73.864	68.710	2.577	-5.368	-7.087	3.098
600	13.382	76.286	69.776	3.906	-5.765	-7.392	2.692
700	13.515	78.360	70.859	5.251	-6.098	-7.637	2.384
717.824	13.531	78.700	71.049	5.492	-6.151	-7.675	2.337

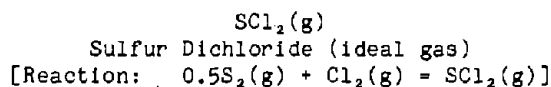
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $C_p^\circ = 13.671 + 0.144 \times 10^{-3}T - 1.378 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 13.671 \times 10^{-3}T + 0.072 \times 10^{-6}T^2 + 1.378 \times 10^2 T^{-1} - 4.545$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -3.070 - 3.330 \times 10^{-3}T + 1.701 \times 10^{-6}T^2 - 86.100T^{-1}$
 $\Delta G_f^\circ = -3.070 + 3.330 \times 10^{-3}T \ln T - 1.701 \times 10^{-6}T^2 - 43.050T^{-1} - 28.107 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -4.185 - 1.067 \times 10^{-3}T - 0.045 \times 10^{-6}T^2 + 69.500T^{-1}$
 $\Delta G_f^\circ = -4.185 + 1.067 \times 10^{-3}T \ln T + 0.045 \times 10^{-6}T^2 + 34.750T^{-1} - 12.924 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -20.343 + 43.673 \times 10^{-3}T - 43.327 \times 10^{-6}T^2 + 1971.700T^{-1}$
 $\Delta G_f^\circ = -20.343 - 43.673 \times 10^{-3}T \ln T + 43.327 \times 10^{-6}T^2 + 985.850T^{-1} + 272.304 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -29.822 + 39.767 \times 10^{-3}T - 23.515 \times 10^{-6}T^2 + 5198.200T^{-1}$
 $\Delta G_f^\circ = -29.822 - 39.767 \times 10^{-3}T \ln T + 23.515 \times 10^{-6}T^2 + 2599.100T^{-1} + 270.457 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
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

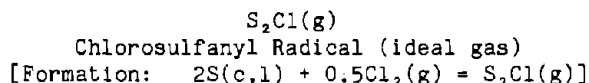
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 13.671 + 0.144 \times 10^{-3}T - 1.378 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 13.671 \times 10^{-3}T + 0.072 \times 10^{-6}T^2 + 1.378 \times 10^{-2}T^{-1} - 4.545$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -19.858 + 0.672 \times 10^{-3}T - 0.176 \times 10^{-6}T^2 + 35.350T^{-1}$
 $\Delta G_r^\circ = -19.858 - 0.672 \times 10^{-3}T \ln T + 0.176 \times 10^{-6}T^2 + 17.675T^{-1} + 17.856 \times 10^{-3}T$

Source: Data from Pankratz (92).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	12.178	69.799	69.799	0	18.800	10.502	-7.698
300	12.194	69.875	69.799	.023	18.795	10.451	-7.613
368.3	12.628	72.428	70.056	.874	18.596	8.571	-5.086
368.3	12.628	72.428	70.056	.874	18.404	8.571	-5.086
388.36	12.755	73.101	70.196	1.128	18.337	8.038	-4.523
388.36	12.755	73.101	70.196	1.128	17.511	8.038	-4.523
400	12.829	73.479	70.286	1.277	17.434	7.755	-4.237
432.02	12.941	74.471	70.560	1.690	17.186	6.989	-3.535
500	13.179	76.383	71.225	2.579	16.436	5.449	-2.382
600	13.386	78.806	72.293	3.908	15.616	3.331	-1.213
700	13.518	80.880	73.374	5.254	14.923	1.340	-.418
717.824	13.534	81.220	73.565	5.495	14.812	.997	-.303

*Data except enthalpy of formation at 298 K estimated.

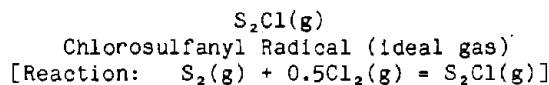
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $\text{Cp}^\circ = 13.672 + 0.144 \times 10^{-3}T - 1.366 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 13.672 \times 10^{-3}T + 0.072 \times 10^{-6}T^2 + 1.366 \times 10^{-2}T^{-1} - 4.541$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta \text{Hf}^\circ = 21.306 - 7.089 \times 10^{-3}T + 3.462 \times 10^{-6}T^2 - 208.750T^{-1}$
 $\Delta \text{Gf}^\circ = 21.306 + 7.089 \times 10^{-3}T \ln T - 3.462 \times 10^{-6}T^2 - 104.375T^{-1} - 74.424 \times 10^{-3}T$
 368.3-388.36 K: $\Delta \text{Hf}^\circ = 19.076 - 2.563 \times 10^{-3}T - 0.030 \times 10^{-6}T^2 + 102.450T^{-1}$
 $\Delta \text{Gf}^\circ = 19.076 + 2.563 \times 10^{-3}T \ln T + 0.030 \times 10^{-6}T^2 + 51.225T^{-1} - 44.059 \times 10^{-3}T$
 388.36-432.02 K: $\Delta \text{Hf}^\circ = -13.241 + 86.916 \times 10^{-3}T - 86.594 \times 10^{-6}T^2 + 3906.850T^{-1}$
 $\Delta \text{Gf}^\circ = -13.241 - 86.916 \times 10^{-3}T \ln T + 86.594 \times 10^{-6}T^2 + 1953.425T^{-1} + 526.398 \times 10^{-3}T$
 432.02-717.824 K: $\Delta \text{Hf}^\circ = -32.198 + 79.105 \times 10^{-3}T - 46.970 \times 10^{-6}T^2 + 10359.850T^{-1}$
 $\Delta \text{Gf}^\circ = -32.198 - 79.105 \times 10^{-3}T \ln T + 46.970 \times 10^{-6}T^2 + 5179.925T^{-1} + 522.703 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	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.

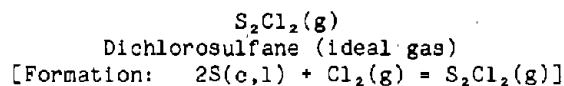
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $\text{Cp}^\circ = 13.672 + 0.144 \times 10^{-3}T - 1.366 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 13.672 \times 10^{-3}T + 0.072 \times 10^{-6}T^2 + 1.366 \times 10^{-2}T^{-1} - 4.541$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta\text{Hr}^\circ = -12.272 + 0.915 \times 10^{-3}T - 0.292 \times 10^{-6}T^2 + 34.150T^{-1}$
 $\Delta\text{Gr}^\circ = -12.272 - 0.915 \times 10^{-3}T \ln T + 0.292 \times 10^{-6}T^2 + 17.075T^{-1} + 17.502 \times 10^{-3}T$

Source: Data from Pankratz (92).



T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	17.392	78.180	78.180	0	-4.000	-6.853	5.023
300	17.419	78.288	78.181	.032	-4.003	-6.870	5.005
368.3	18.097	81.938	78.548	1.248	-4.119	-7.512	4.458
368.3	18.097	81.938	78.548	1.248	-4.311	-7.512	4.458
388.36	18.296	82.903	78.749	1.613	-4.352	-7.684	4.324
388.36	18.296	82.903	78.749	1.613	-5.178	-7.684	4.324
400	18.411	83.445	78.878	1.827	-5.238	-7.759	4.239
432.02	18.588	84.870	79.270	2.419	-5.443	-7.954	4.024
500	18.965	87.617	80.221	3.698	-6.094	-8.291	3.624
600	19.316	91.107	81.752	5.613	-6.762	-8.664	3.156
700	19.560	94.104	83.308	7.557	-7.296	-8.938	2.791
717.824	19.592	94.596	83.582	7.906	-7.378	-8.978	2.733

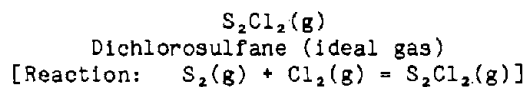
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-1500 K: $C_p^\circ = 19.397 + 0.706 \times 10^{-3}T - 1.969 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 19.397 \times 10^{-3}T + 0.353 \times 10^{-6}T^2 + 1.969 \times 10^{-2}T^{-1} - 6.475$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -1.994 - 5.778 \times 10^{-3}T + 3.699 \times 10^{-6}T^2 - 182.600T^{-1}$
 $\Delta G_f^\circ = -1.994 + 5.778 \times 10^{-3}T \ln T - 3.699 \times 10^{-6}T^2 - 91.300T^{-1} - 47.088 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -4.224 - 1.252 \times 10^{-3}T + 0.207 \times 10^{-6}T^2 + 128.600T^{-1}$
 $\Delta G_f^\circ = -4.224 + 1.252 \times 10^{-3}T \ln T - 0.207 \times 10^{-6}T^2 + 64.300T^{-1} - 16.722 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -36.541 + 88.228 \times 10^{-3}T - 86.357 \times 10^{-6}T^2 + 3933.000T^{-1}$
 $\Delta G_f^\circ = -36.541 - 88.228 \times 10^{-3}T \ln T + 86.357 \times 10^{-6}T^2 + 1966.500T^{-1} + 553.734 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -55.498 + 80.416 \times 10^{-3}T - 46.733 \times 10^{-6}T^2 + 10386.000T^{-1}$
 $\Delta G_f^\circ = -55.498 - 80.416 \times 10^{-3}T \ln T + 46.733 \times 10^{-6}T^2 + 5193.000T^{-1} + 550.040 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log K _r
	C _p ^o	S ^o	-(G ^o - H ₂₉₈ ^o)/T	H ^o - H ₂₉₈ ^o	ΔH _r ^o	ΔG _r ^o	
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

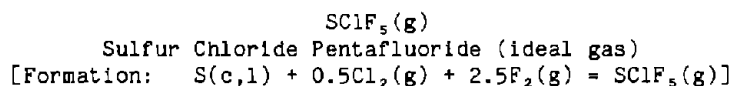
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1500 K: $C_p^o = 19.397 + 0.706 \times 10^{-3}T - 1.969 \times 10^{-5}T^2$
 $H^o - H_{298}^o = 19.397 \times 10^{-3}T + 0.353 \times 10^{-6}T^2 + 1.969 \times 10^{-2}T^3 - 6.475$

Reaction equations (kcal/mol):

298.15-1500 K: $\Delta H_r^o = -35.571 + 2.227 \times 10^{-3}T - 0.055 \times 10^{-6}T^2 + 60.300T^{-1}$
 $\Delta G_r^o = -35.571 - 2.227 \times 10^{-3}T \ln T + 0.055 \times 10^{-6}T^2 + 30.150T^{-1} + 44.838 \times 10^{-3}T$

Source: Data from Pankratz (92).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H° ₂₉₈)/T	H°- H° ₂₉₈	ΔHf°	ΔGf°	
298.15	24.938	76.439	76.439	0	-248.300	-224.754	164.747
300	25.036	76.593	76.440	.046	-248.307	-224.608	163.625
368.3	27.858	82.057	76.982	1.869	-248.452	-219.194	130.068
368.3	27.858	82.057	76.982	1.869	-248.548	-219.194	130.068
388.36	28.687	83.557	77.283	2.436	-248.575	-217.594	122.450
388.36	28.687	83.557	77.283	2.436	-248.988	-217.594	122.450
400	29.168	84.411	77.479	2.773	-249.017	-216.653	118.372
432.02	29.979	86.688	78.078	3.720	-249.104	-214.059	108.287
500	31.701	91.214	79.560	5.827	-249.337	-208.522	91.144
600	33.305	97.146	82.008	9.083	-249.447	-200.346	72.975
700	34.367	102.365	84.551	12.470	-249.419	-192.163	59.995
717.824	34.497	103.231	85.004	13.084	-249.403	-190.705	58.062

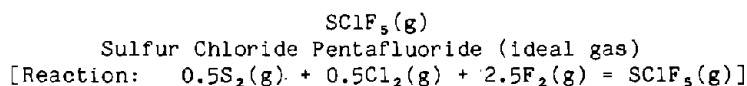
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 34.913 + 1.650x10⁻³T - 9.304x10⁻⁵T²
H°- H°₂₉₈ = 34.913x10⁻³T + 0.825x10⁻⁶T² + 9.304x10⁻²T⁻¹ - 13.603

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -250.440 + 1.055x10⁻³T + 2.063x10⁻⁶T² + 489.400T⁻¹
ΔGf° = -250.440 - 1.055x10⁻³TlnT - 2.063x10⁻⁶T² + 244.700T⁻¹ + 90.027x10⁻³T
368.3-388.36 K: ΔHf° = -251.555 + 3.318x10⁻³T + 0.317x10⁻⁶T² + 645.000T⁻¹
ΔGf° = -251.555 - 3.318x10⁻³TlnT - 0.317x10⁻⁶T² + 322.500T⁻¹ + 105.210x10⁻³T
388.36-432.02 K: ΔHf° = -267.713 + 48.058x10⁻³T - 42.965x10⁻⁶T² + 2547.200T⁻¹
ΔGf° = -267.713 - 48.058x10⁻³TlnT + 42.965x10⁻⁶T² + 1273.600T⁻¹ + 390.438x10⁻³T
432.02-717.824 K: ΔHf° = -277.192 + 44.153x10⁻³T - 23.153x10⁻⁶T² + 5773.700T⁻¹
ΔGf° = -277.192 - 44.153x10⁻³TlnT + 23.153x10⁻⁶T² + 2886.850T⁻¹ + 388.590x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	24.938	76.439	76.439	0	-263.655	-234.267	171.720
300	25.036	76.593	76.440	.046	-263.659	-234.085	170.529
400	29.168	84.411	77.479	2.773	-263.668	-224.218	122.506
500	31.701	91.214	79.560	5.827	-263.464	-214.375	93.702
600	33.305	97.146	82.008	9.083	-263.142	-204.587	74.520
700	34.367	102.365	84.551	12.470	-262.744	-194.858	60.837
800	35.099	107.005	87.072	15.946	-262.302	-185.192	50.591
900	35.621	111.171	89.523	19.483	-261.827	-175.579	42.636
1000	36.006	114.944	91.879	23.065	-261.336	-166.025	36.284
1100	36.296	118.390	94.135	26.681	-260.831	-156.516	31.096
1200	36.521	121.559	96.291	30.322	-260.318	-147.057	26.782
1300	36.698	124.489	98.347	33.984	-259.799	-137.637	23.139
1400	36.840	127.214	100.313	37.661	-259.283	-128.262	20.022
1500	36.955	129.760	102.193	41.351	-258.765	-118.922	17.327
1600	37.050	132.148	103.991	45.051	-258.250	-109.615	14.973
1700	37.129	134.397	105.715	48.760	-257.734	-100.339	12.899
1800	37.196	136.521	107.367	52.477	-257.225	-91.096	11.060
2000	37.301	140.446	110.482	59.927	-256.217	-72.691	7.943

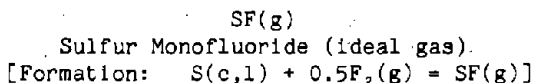
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 34.913 + 1.650 \times 10^{-3}T - 9.304 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 34.913 \times 10^{-3}T + 0.825 \times 10^{-6}T^2 + 9.304 \times 10^{-2}T^3 - 13.603$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -267.228 + 5.058 \times 10^{-3}T + 0.186 \times 10^{-6}T^2 + 610.850T^{-1}$
 $\Delta G_r^\circ = -267.228 - 5.058 \times 10^{-3}T \ln T - 0.186 \times 10^{-6}T^2 + 305.425T^{-1} + 135.990 \times 10^{-3}T$

Source: Data from Chase (17).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	8.401	53.815	53.815	0	3.100	-3.439	2.521
300	8.407	53.867	53.815	.016	3.099	-3.479	2.535
368.3	8.550	55.608	53.990	.596	3.034	-4.971	2.950
368.3	8.550	55.608	53.990	.596	2.938	-4.971	2.950
388.36	8.593	56.063	54.086	.768	2.913	-5.400	3.039
388.36	8.593	56.063	54.086	.768	2.500	-5.400	3.039
400	8.617	56.317	54.147	.868	2.467	-5.637	3.080
432.02	8.655	56.982	54.333	1.145	2.353	-6.282	3.178
500	8.737	58.254	54.782	1.736	1.996	-7.610	3.326
600	8.813	59.854	55.497	2.614	1.602	-9.492	3.457
700	8.864	61.217	56.220	3.498	1.261	-11.314	3.532
717.824	8.871	61.440	56.347	3.656	1.206	-11.633	3.542

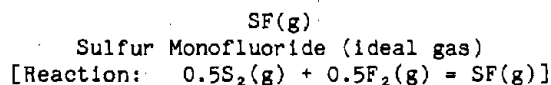
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 8.853 + 0.134x10⁻³T - 0.438x10⁻⁵T²
H° - H₂₉₈° = 8.853x10⁻³T + 0.067x10⁻⁶T² + 0.438x10⁻²T⁻¹ - 2.792

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 4.559 - 3.575x10⁻³T + 1.697x10⁻⁶T² - 162.050T⁻¹
ΔGf° = 4.559 + 3.575x10⁻³T ln T - 1.697x10⁻⁶T² - 81.025T⁻¹ - 45.776x10⁻³T
368.3-388.36 K: ΔHf° = 3.443 - 1.312x10⁻³T - 0.049x10⁻⁶T² - 6.450T⁻¹
ΔGf° = 3.443 + 1.312x10⁻³T ln T + 0.049x10⁻⁶T² - 3.225T⁻¹ - 30.593x10⁻³T
388.36-432.02 K: ΔHf° = -12.715 + 43.428x10⁻³T - 43.331x10⁻⁶T² + 1895.750T⁻¹
ΔGf° = -12.715 - 43.428x10⁻³T ln T + 43.331x10⁻⁶T² + 947.875T⁻¹ + 254.635x10⁻³T
432.02-717.824 K: ΔHf° = -22.194 + 39.522x10⁻³T - 23.519x10⁻⁶T² + 5122.250T⁻¹
ΔGf° = -22.194 - 39.522x10⁻³T ln T + 23.519x10⁻⁶T² + 2561.125T⁻¹ + 252.788x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H 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

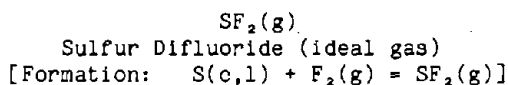
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 8.853 + 0.134 \times 10^{-3}T - 0.438 \times 10^{-6}T^2$
 $H^\circ - H_{298}^\circ = 8.853 \times 10^{-3}T + 0.067 \times 10^{-6}T^2 + 0.438 \times 10^{-2}T^{-1} - 2.792$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -12.230 + 0.427 \times 10^{-3}T - 0.180 \times 10^{-6}T^2 - 40.600T^{-1}$
 $\Delta G_r^\circ = -12.230 - 0.427 \times 10^{-3}T \ln T + 0.180 \times 10^{-6}T^2 - 20.300T^{-1} + 0.187 \times 10^{-3}T$

Source: Data from Pankratz (92).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	10.733	61.565	61.565	0	-70.900	-72.528	53.164
300	10.753	61.632	61.565	.020	-70.904	-72.538	52.844
368.3	11.390	63.909	61.794	.779	-71.050	-72.895	43.255
368.3	11.390	63.909	61.794	.779	-71.146	-72.895	43.255
388.36	11.577	64.518	61.919	1.010	-71.191	-72.988	41.074
388.36	11.577	64.518	61.919	1.010	-71.604	-72.988	41.074
400	11.686	64.862	62.000	1.145	-71.648	-73.029	39.901
432.02	11.885	65.770	62.246	1.522	-71.788	-73.135	36.997
500	12.307	67.541	62.847	2.347	-72.187	-73.313	32.044
600	12.717	69.824	63.826	3.599	-72.622	-73.496	26.771
700	12.995	71.806	64.826	4.886	-72.983	-73.612	22.982
717.824	13.029	72.133	65.003	5.118	-73.041	-73.626	22.416

*Data except enthalpy of formation at 298 K estimated.

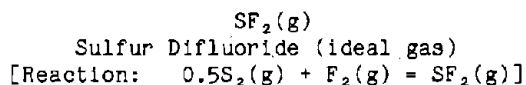
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 12.941 + 0.578x10⁻³T - 2.116x10⁻⁵T⁻²
H° - H°₂₉₈ = 12.941x10⁻³T + 0.289x10⁻⁶T² + 2.116x10⁻²T⁻¹ - 4.594

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -69.798 - 3.741x10⁻³T + 1.832x10⁻⁶T² - 44.500T⁻¹
ΔGf° = -69.798 + 3.741x10⁻³TlnT - 1.832x10⁻⁶T² - 22.250T⁻¹ - 29.675x10⁻³T
368.3-388.36 K: ΔHf° = -70.913 - 1.478x10⁻³T + 0.086x10⁻⁶T² + 111.100T⁻¹
ΔGf° = -70.913 + 1.478x10⁻³TlnT - 0.086x10⁻⁶T² + 55.550T⁻¹ - 14.492x10⁻³T
388.36-432.02 K: ΔHf° = -87.072 + 43.262x10⁻³T - 43.196x10⁻⁶T² + 2013.300T⁻¹
ΔGf° = -87.072 - 43.262x10⁻³TlnT + 43.196x10⁻⁶T² + 1006.650T⁻¹ + 270.737x10⁻³T
432.02-717.824 K: ΔHf° = -96.550 + 39.356x10⁻³T - 23.384x10⁻⁶T² + 5239.800T⁻¹
ΔGf° = -96.550 - 39.356x10⁻³TlnT + 23.384x10⁻⁶T² + 2619.900T⁻¹ + 268.889x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H 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: $C_p^\circ = 12.941 + 0.578 \times 10^{-3}T - 2.116 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 12.941 \times 10^{-3}T + 0.289 \times 10^{-6}T^2 + 2.116 \times 10^{-2}T^{-1} - 4.594$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -86.587 + 0.261 \times 10^{-3}T - 0.045 \times 10^{-6}T^2 + 76.950T^{-1}$
 $\Delta G_r^\circ = -86.587 - 0.261 \times 10^{-3}T \ln T + 0.045 \times 10^{-6}T^2 + 38.475T^{-1} + 16.288 \times 10^{-5}T$

Source: Data from Pankratz (92).

SF₃(g)
Sulfur Trifluoride (ideal gas)
[Formation: S(c,l) + 1.5F₂(g) = SF₃(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	13.773	66.347	66.347	0	-120.400	-116.232	85.199
300	13.813	66.432	66.347	.026	-120.405	-116.206	84.655
368.3	15.025	69.402	66.644	1.016	-120.581	-115.231	68.378
368.3	15.025	69.402	66.644	1.016	-120.677	-115.231	68.378
388.36	15.381	70.209	66.808	1.321	-120.726	-114.933	64.678
388.36	15.381	70.209	66.808	1.321	-121.139	-114.933	64.678
400	15.588	70.666	66.913	1.501	-121.184	-114.746	62.694
432.02	15.966	71.881	67.237	2.006	-121.322	-114.226	57.784
500	16.769	74.280	68.034	3.123	-121.704	-113.076	49.425
600	17.554	77.411	69.341	4.842	-122.088	-111.312	40.545
700	18.088	80.160	70.694	6.626	-122.376	-109.493	34.185
717.824	18.155	80.616	70.935	6.949	-122.419	-109.164	33.236

*Data except enthalpy of formation at 298 K estimated.

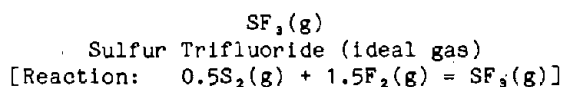
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 17.955 + 1.138x10⁻³T - 4.019x10⁻⁵T⁻²
H° - H°₂₉₈ = 17.955x10⁻³T + 0.569x10⁻⁶T² + 4.019x10⁻²T⁻¹ - 6.752

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -120.012 - 2.981x10⁻³T + 2.025x10⁻⁶T² + 95.550T⁻¹
ΔGf° = -120.012 + 2.981x10⁻³T lnT - 2.025x10⁻⁶T² + 47.775T⁻¹ - 4.242x10⁻³T
368.3-388.36 K: ΔHf° = -121.127 - 0.718x10⁻³T + 0.279x10⁻⁶T² + 251.150T⁻¹
ΔGf° = -121.127 + 0.718x10⁻³T lnT - 0.279x10⁻⁶T² + 125.575T⁻¹ + 10.941x10⁻³T
388.36-432.02 K: ΔHf° = -137.285 + 44.022x10⁻³T - 43.003x10⁻⁶T² + 2153.350T⁻¹
ΔGf° = -137.285 - 44.022x10⁻³T lnT + 43.003x10⁻⁶T² + 1076.675T⁻¹ + 296.169x10⁻³T
432.02-717.824 K: ΔHf° = -146.764 + 40.116x10⁻³T - 23.191x10⁻⁶T² + 5379.850T⁻¹
ΔGf° = -146.764 - 40.116x10⁻³T lnT + 23.191x10⁻⁶T² + 2689.925T⁻¹ + 294.322x10⁻³T



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: $C_p^\circ = 17.955 + 1.138 \times 10^{-3}T - 4.019 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 17.955 \times 10^{-3}T + 0.569 \times 10^{-6}T^2 + 4.019 \times 10^{-2}T^{-1} - 6.752$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -136.801 + 1.021 \times 10^{-3}T + 0.148 \times 10^{-6}T^2 + 217.000T^{-1}$
 $\Delta G_r^\circ = -136.801 - 1.021 \times 10^{-3}T \ln T - 0.148 \times 10^{-6}T^2 + 108.500T^{-1} + 41.721 \times 10^{-3}T$

Source: Data from Pankratz (92).

SF₄(g)
Sulfur Tetrafluoride (ideal gas)
[Formation: S(c,l) + 2F₂(g) = SF₄(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	18.546	71.590	71.590	0	-182.400	-172.574	126.498
300	18.600	71.704	71.591	.034	-182.404	-172.513	125.674
368.3	20.179	75.702	71.988	1.368	-182.496	-170.249	101.025
368.3	20.179	75.702	71.988	1.368	-182.592	-170.249	101.025
388.36	20.643	76.784	72.208	1.777	-182.615	-169.576	95.428
388.36	20.643	76.784	72.208	1.777	-183.028	-169.576	95.428
400	20.912	77.398	72.351	2.019	-183.057	-169.173	92.430
432.02	21.372	79.026	72.786	2.696	-183.151	-168.058	85.016
500	22.348	82.231	73.855	4.188	-183.433	-165.657	72.408
600	23.265	86.393	75.606	6.472	-183.666	-162.079	59.036
700	23.874	90.028	77.412	8.831	-183.803	-158.469	49.475
717.824	23.949	90.629	77.733	9.257	-183.819	-157.823	48.051

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 23.999 + 1.094x10⁻³T - 5.137x10⁻⁵T⁻²
H° - H₂₉₈° = 23.999x10⁻³T + 0.547x10⁻⁶T² + 5.137x10⁻²T⁻¹ - 8.927

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -182.742 - 1.191x10⁻³T + 1.916x10⁻⁶T² + 157.100T⁻¹
ΔGf° = -182.742 + 1.191x10⁻³TlnT - 1.916x10⁻⁶T² + 78.550T⁻¹ + 27.006x10⁻³T
368.3-388.36 K: ΔHf° = -183.857 + 1.072x10⁻³T + 0.170x10⁻⁶T² + 312.700T⁻¹
ΔGf° = -183.857 - 1.072x10⁻³TlnT - 0.170x10⁻⁶T² + 156.350T⁻¹ + 42.189x10⁻³T
388.36-432.02 K: ΔHf° = -200.016 + 45.812x10⁻³T - 43.112x10⁻⁶T² + 2214.900T⁻¹
ΔGf° = -200.016 - 45.812x10⁻³TlnT + 43.112x10⁻⁶T² + 1107.450T⁻¹ + 327.417x10⁻³T
432.02-717.824 K: ΔHf° = -209.494 + 41.906x10⁻³T - 23.300x10⁻⁶T² + 5441.400T⁻¹
ΔGf° = -209.494 - 41.906x10⁻³TlnT + 23.300x10⁻⁶T² + 2720.700T⁻¹ + 325.570x10⁻³T

SF₄(g)
Sulfur Tetrafluoride (ideal gas)
[Reaction: 0.5S₂(g) + 2F₂(g) = SF₄(g)]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H _{2,98} °)/T	H°- H _{2,98} °	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

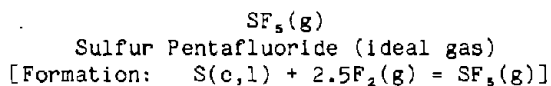
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 23.999 + 1.094 \times 10^{-3}T - 5.137 \times 10^{-5}T^2$
 $H^\circ - H_{2,98}^\circ = 23.999 \times 10^{-3}T + 0.547 \times 10^{-6}T^2 + 5.137 \times 10^{-2}T^{-1} - 8.927$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -199.531 + 2.811 \times 10^{-3}T + 0.039 \times 10^{-6}T^2 + 278.550T^{-1}$
 $\Delta G_r^\circ = -199.531 - 2.811 \times 10^{-3}T \ln T + 0.039 \times 10^{-6}T^2 + 139.275T^{-1} + 72.969 \times 10^{-3}T$

Source: Data from Pankratz (92).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H _{2,98} °)/T	H° - H _{2,98} °	ΔHf°	ΔGf°	
298.15*	21.425	72.811	72.811	0	-217.100	-200.416	146.907
300	21.507	72.944	72.811	.040	-217.105	-200.313	145.926
368.3	23.862	77.631	73.275	1.604	-217.227	-196.473	116.586
368.3	23.862	77.631	73.275	1.604	-217.323	-196.473	116.586
388.36	24.554	78.915	73.534	2.090	-217.348	-195.337	109.924
388.36	24.554	78.915	73.534	2.090	-217.761	-195.337	109.924
400	24.955	79.646	73.701	2.378	-217.790	-194.664	106.358
432.02	25.617	81.593	74.215	3.188	-217.878	-192.810	97.537
500	27.021	85.456	75.486	4.985	-218.130	-188.843	82.542
600	28.309	90.505	77.578	7.756	-218.291	-182.969	66.645
700	29.152	94.936	79.747	10.632	-218.335	-177.077	55.285
717.824	29.255	95.670	80.134	11.152	-218.333	-176.026	53.593

*Data except enthalpy of formation at 298 K estimated.

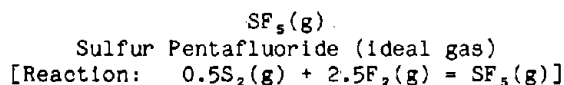
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 29.716 + 1.224x10⁻³T - 7.694x10⁻⁵T⁻²
H° - H_{2,98}° = 29.716x10⁻³T + 0.612x10⁻⁶T² + 7.694x10²T⁻¹ - 11.495

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -218.565 + 0.272x10⁻³T + 1.894x10⁻⁶T² + 362.550T⁻¹
ΔGf° = -218.565 - 0.272x10⁻³T ln T - 1.894x10⁻⁶T² + 181.275T⁻¹ + 60.948x10⁻³T
368.3-388.36 K: ΔHf° = -219.681 + 2.535x10⁻³T + 0.148x10⁻⁶T² + 518.150T⁻¹
ΔGf° = -219.681 - 2.535x10⁻³T ln T - 0.148x10⁻⁶T² + 259.075T⁻¹ + 76.131x10⁻³T
388.36-432.02 K: ΔHf° = -235.839 + 47.275x10⁻³T - 43.134x10⁻⁶T² + 2420.350T⁻¹
ΔGf° = -235.839 - 47.275x10⁻³T ln T + 43.134x10⁻⁶T² + 1210.175T⁻¹ + 361.359x10⁻³T
432.02-717.824 K: ΔHf° = -245.318 + 43.369x10⁻³T - 23.322x10⁻⁶T² + 5646.850T⁻¹
ΔGf° = -245.318 - 43.369x10⁻³T ln T + 23.322x10⁻⁶T² + 2823.425T⁻¹ + 359.512x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H 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.

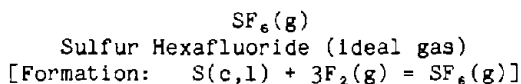
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 29.716 + 1.224 \times 10^{-3}T - 7.694 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 29.716 \times 10^{-3}T + 0.612 \times 10^{-6}T^2 + 7.694 \times 10^{-2}T^{-1} - 11.495$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -235.354 + 4.274 \times 10^{-3}T + 0.017 \times 10^{-6}T^2 + 484.000T^{-1}$
 $\Delta G_r^\circ = -235.354 - 4.274 \times 10^{-3}T \ln T - 0.017 \times 10^{-6}T^2 + 242.000T^{-1} + 106.911 \times 10^{-3}T$

Source: Data from Pankratz (92).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	23.174	69.651	69.651	0	-291.700	-266.852	195.606
300	23.278	69.795	69.652	.043	-291.709	-266.699	194.288
368.3	26.375	74.925	70.157	1.756	-291.943	-260.975	154.861
368.3	26.375	74.925	70.157	1.756	-292.039	-260.975	154.861
388.36	27.285	76.348	70.441	2.294	-292.089	-259.281	145.909
388.36	27.285	76.348	70.441	2.294	-292.502	-259.281	145.909
400	27.813	77.162	70.625	2.615	-292.544	-258.285	141.119
432.02	28.730	79.339	71.191	3.520	-292.664	-255.539	129.270
500	30.676	83.700	72.600	5.550	-292.958	-249.670	109.129
600	32.521	89.468	74.941	8.716	-293.139	-240.994	87.781
700	33.754	94.580	77.389	12.034	-293.165	-232.299	72.526
717.824	33.906	95.430	77.826	12.637	-293.157	-230.749	70.254

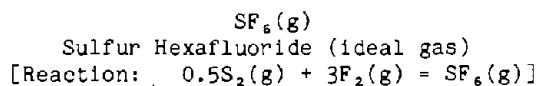
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 33.865 + 2.318x10⁻³T - 10.118x10⁻⁵T⁻²
H° - H₂₉₈° = 33.865x10⁻³T + 1.159x10⁻⁶T² + 10.118x10⁻²T⁻¹ - 13.593

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -293.820 + 0.167x10⁻³T + 2.354x10⁻⁶T² + 554.700T⁻¹
ΔGf° = -293.820 - 0.167x10⁻³TlnT - 2.354x10⁻⁶T² + 277.350T⁻¹ + 88.981x10⁻³T
368.3-388.36 K: ΔHf° = -294.935 + 2.430x10⁻³T + 0.608x10⁻⁶T² + 710.300T⁻¹
ΔGf° = -294.935 - 2.430x10⁻³TlnT - 0.608x10⁻⁶T² + 355.150T⁻¹ + 104.164x10⁻³T
388.36-432.02 K: ΔHf° = -311.093 + 47.170x10⁻³T - 42.674x10⁻⁶T² + 2612.500T⁻¹
ΔGf° = -311.093 - 47.170x10⁻³TlnT + 42.674x10⁻⁶T² + 1306.250T⁻¹ + 389.393x10⁻³T
432.02-717.824 K: ΔHf° = -320.572 + 43.264x10⁻³T - 22.862x10⁻⁶T² + 5839.000T⁻¹
ΔGf° = -320.572 - 43.264x10⁻³TlnT + 22.862x10⁻⁶T² + 2919.500T⁻¹ + 387.545x10⁻³T



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

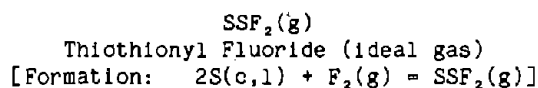
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 33.865 + 2.318 \times 10^{-3}T - 10.118 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 33.865 \times 10^{-3}T + 1.159 \times 10^{-6}T^2 + 10.118 \times 10^{-2}T^{-1} - 13.593$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -310.608 + 4.169 \times 10^{-3}T + 0.477 \times 10^{-6}T^2 + 676.150T^{-1}$
 $\Delta G_r^\circ = -310.608 - 4.169 \times 10^{-3}T \ln T - 0.477 \times 10^{-6}T^2 + 338.075T^{-1} + 134.944 \times 10^{-3}T$

Source: Data from Pankratz (92).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	15.088	69.960	69.960	0	-95.900	-97.747	71.650
300	15.125	70.053	69.960	.028	-95.906	-97.758	71.216
368.3	16.202	73.282	70.283	1.104	-96.119	-98.157	58.246
368.3	16.202	73.282	70.283	1.104	-96.311	-98.157	58.246
388.36	16.518	74.149	70.460	1.433	-96.377	-98.255	55.292
388.36	16.518	74.149	70.460	1.433	-97.203	-98.255	55.292
400	16.702	74.640	70.575	1.626	-97.277	-98.286	53.700
432.02	17.007	75.938	70.925	2.166	-97.517	-98.358	49.757
500	17.655	78.478	71.782	3.348	-98.233	-98.429	43.023
600	18.252	81.753	73.178	5.145	-98.980	-98.394	35.840
700	18.643	84.598	74.611	6.991	-99.582	-98.248	30.674
717.824	18.691	85.067	74.865	7.324	-99.676	-98.212	29.901

*Enthalpy of formation at 298 K estimated.

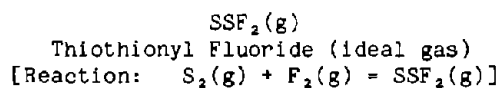
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 18.814 + 0.634x10⁻³T - 3.480x10⁻⁵T²
 H° - H°₂₉₈ = 18.814x10⁻³T + 0.317x10⁻⁶T² + 3.480x10⁻²T³ - 6.805

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -94.203 - 6.042x10⁻³T + 3.577x10⁻⁶T² - 63.700T⁻¹
 ΔGf° = -94.203 + 6.042x10⁻³T ln T - 3.577x10⁻⁶T² - 31.850T⁻¹ - 44.887x10⁻³T
 368.3-388.36 K: ΔHf° = -96.433 - 1.516x10⁻³T + 0.085x10⁻⁶T² + 247.500T⁻¹
 ΔGf° = -96.433 + 1.516x10⁻³T ln T - 0.085x10⁻⁶T² + 123.750T⁻¹ - 14.521x10⁻³T
 388.36-432.02 K: ΔHf° = -128.750 + 87.964x10⁻³T - 86.479x10⁻⁶T² + 4051.900T⁻¹
 ΔGf° = -128.750 - 87.964x10⁻³T ln T + 86.479x10⁻⁶T² + 2025.950T⁻¹ + 555.935x10⁻³T
 432.02-717.824 K: ΔHf° = -147.707 + 80.152x10⁻³T - 46.855x10⁻⁶T² + 10504.900T⁻¹
 ΔGf° = -147.707 - 80.152x10⁻³T ln T + 46.855x10⁻⁶T² + 5252.450T⁻¹ + 552.241x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/T$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔH°	ΔG°	
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.

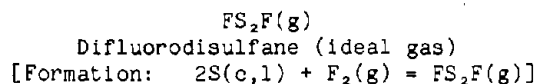
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $\text{Cp}^\circ = 18.814 + 0.634 \times 10^{-3}T - 3.480 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 18.814 \times 10^{-3}T + 0.317 \times 10^{-6}T^2 + 3.480 \times 10^{-2}T^{-1} - 6.805$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta \text{H}^\circ = -127.781 + 1.963 \times 10^{-3}T - 0.177 \times 10^{-6}T^2 + 179.200T^{-1}$
 $\Delta \text{G}^\circ = -127.781 - 1.963 \times 10^{-3}T \ln T + 0.177 \times 10^{-6}T^2 + 89.600T^{-1} + 47.039 \times 10^{-3}T$

Source: Data from Pankratz (92).



T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15*	15.784	70.260	70.260	0	-80.400	-82.336	60.353
300	15.817	70.358	70.261	.029	-80.405	-82.349	59.990
368.3	16.763	73.714	70.598	1.148	-80.575	-82.773	49.117
368.3	16.763	73.714	70.598	1.148	-80.767	-82.773	49.117
388.36	17.041	74.610	70.782	1.487	-80.823	-82.880	46.640
388.36	17.041	74.610	70.782	1.487	-81.649	-82.880	46.640
400	17.202	75.116	70.901	1.686	-81.717	-82.916	45.303
432.02	17.464	76.451	71.263	2.241	-81.942	-83.005	41.990
500	18.020	79.050	72.148	3.451	-82.630	-83.112	36.328
600	18.525	82.383	73.583	5.280	-83.345	-83.137	30.282
700	18.853	85.265	75.051	7.150	-83.923	-83.056	25.931
717.824	18.893	85.739	75.310	7.486	-84.013	-83.031	25.280

*Enthalpy of formation at 298 K estimated.

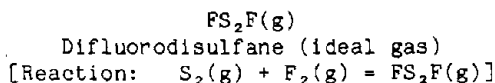
Phase changes: 368.3 K, orthorhombic $\rightarrow$ monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second-order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $C_p^\circ = 19.051 + 0.494 \times 10^{-3}T - 3.035 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 19.051 \times 10^{-3}T + 0.247 \times 10^{-6}T^2 + 3.035 \times 10^{-2}T^{-1} - 6.720$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -78.618 - 5.805 \times 10^{-3}T + 3.507 \times 10^{-6}T^2 - 108.200T^{-1}$
 $\Delta G_f^\circ = -78.618 + 5.805 \times 10^{-3}T \ln T - 3.507 \times 10^{-6}T^2 - 54.100T^{-1} - 43.892 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -80.848 - 1.279 \times 10^{-3}T + 0.015 \times 10^{-6}T^2 + 203.000T^{-1}$
 $\Delta G_f^\circ = -80.848 + 1.279 \times 10^{-3}T \ln T - 0.015 \times 10^{-6}T^2 + 101.500T^{-1} - 13.526 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -113.165 + 88.201 \times 10^{-3}T - 86.549 \times 10^{-6}T^2 + 4007.400T^{-1}$
 $\Delta G_f^\circ = -113.165 - 88.201 \times 10^{-3}T \ln T + 86.549 \times 10^{-6}T^2 + 2003.700T^{-1} + 556.931 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -132.122 + 80.389 \times 10^{-3}T - 46.925 \times 10^{-6}T^2 + 10460.400T^{-1}$
 $\Delta G_f^\circ = -132.122 - 80.389 \times 10^{-3}T \ln T + 46.925 \times 10^{-6}T^2 + 5230.200T^{-1} + 553.236 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
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.

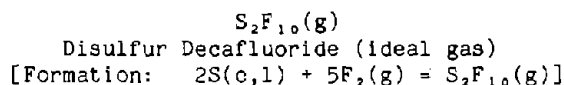
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 19.051 + 0.494 \times 10^{-3}T - 3.035 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 19.051 \times 10^{-3}T + 0.247 \times 10^{-6}T^2 + 3.035 \times 10^{-2}T^{-1} - 6.720$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -112.196 + 2.200 \times 10^{-3}T - 0.247 \times 10^{-6}T^2 + 134.700T^{-1}$
 $\Delta G_r^\circ = -112.196 - 2.200 \times 10^{-3}T \ln T + 0.247 \times 10^{-6}T^2 + 67.350T^{-1} + 48.034 \times 10^{-3}T$

Source: Data from Pankratz (92).



T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	42.228	94.872	94.872	0	-493.400	-444.901	326.117
300	42.417	95.133	94.873	.078	-493.412	-444.601	323.888
368.3	47.958	104.469	95.794	3.195	-493.668	-433.454	257.209
368.3	47.958	104.469	95.794	3.195	-493.860	-433.454	257.209
388.36	49.586	107.057	96.311	4.173	-493.902	-430.161	242.070
388.36	49.586	107.057	96.311	4.173	-494.728	-430.161	242.070
400	50.530	108.535	96.645	4.756	-494.779	-428.226	233.969
432.02	52.161	112.489	97.675	6.400	-494.931	-422.894	213.930
500	55.625	120.400	100.234	10.083	-495.346	-411.516	179.871
600	58.900	130.851	104.484	15.820	-495.473	-394.734	143.780
700	61.072	140.105	108.925	21.826	-495.307	-377.954	118.001
717.824	61.338	141.644	109.718	22.917	-495.253	-374.966	114.162

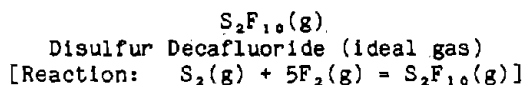
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $C_p^\circ = 61.800 + 3.424 \times 10^{-3}T - 18.305 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 61.800 \times 10^{-3}T + 1.712 \times 10^{-6}T^2 + 18.305 \times 10^{-2}T^{-1} - 24.717$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -498.059 + 2.912 \times 10^{-3}T + 4.276 \times 10^{-6}T^2 + 1016.800T^{-1}$
 $\Delta G_f^\circ = -498.059 - 2.912 \times 10^{-3}T \ln T - 4.276 \times 10^{-6}T^2 + 508.400T^{-1} + 190.437 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -500.289 + 7.438 \times 10^{-3}T + 0.784 \times 10^{-6}T^2 + 1328.000T^{-1}$
 $\Delta G_f^\circ = -500.289 - 7.438 \times 10^{-3}T \ln T - 0.784 \times 10^{-6}T^2 + 664.000T^{-1} + 220.803 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -532.606 + 96.918 \times 10^{-3}T - 85.780 \times 10^{-6}T^2 + 5132.400T^{-1}$
 $\Delta G_f^\circ = -532.606 - 96.918 \times 10^{-3}T \ln T + 85.780 \times 10^{-6}T^2 + 2566.200T^{-1} + 791.260 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -551.563 + 89.106 \times 10^{-3}T - 46.156 \times 10^{-6}T^2 + 11585.400T^{-1}$
 $\Delta G_f^\circ = -551.563 - 89.106 \times 10^{-3}T \ln T + 46.156 \times 10^{-6}T^2 + 5792.700T^{-1} + 787.565 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
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: $C_p^\circ = 61.800 + 3.424 \times 10^{-3}T - 18.305 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 61.800 \times 10^{-3}T + 1.712 \times 10^{-6}T^2 + 18.305 \times 10^2 T^{-1} - 24.717$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -531.636 + 10.917 \times 10^{-3}T + 0.522 \times 10^{-6}T^2 + 1259.700T^{-1}$
 $\Delta G_r^\circ = -531.636 - 10.917 \times 10^{-3}T \ln T - 0.522 \times 10^{-6}T^2 + 629.850T^{-1} + 282.363 \times 10^{-3}T$

Source: Data from Pankratz (92).

SO(g)
Sulfur Monoxide (ideal gas)
[Formation: $S(c,l) + 0.5O_2(g) = SO(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H _{2,98} °)/T	H°- H _{2,98} °	ΔHf°	ΔGf°	
298.15	7.212	53.020	53.020	0	1.200	-5.018	3.679
300	7.217	53.064	53.021	.013	1.197	-5.057	3.684
368.3	7.440	54.566	53.172	.514	1.072	-6.468	3.838
368.3	7.440	54.566	53.172	.514	.976	-6.468	3.838
388.36	7.505	54.963	53.255	.663	.935	-6.872	3.867
388.36	7.505	54.963	53.255	.663	.522	-6.872	3.867
400	7.543	55.185	53.308	.751	.480	-7.093	3.875
432.02	7.640	55.770	53.469	.994	.344	-7.694	3.892
500	7.846	56.901	53.859	1.521	-.053	-8.925	3.901
600	8.087	58.354	54.491	2.318	-.490	-10.657	3.882
700	8.273	59.615	55.134	3.137	-.860	-12.320	3.846
717.824	8.298	59.823	55.247	3.285	-.920	-12.611	3.839

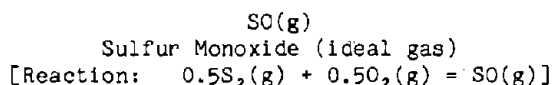
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: $C_p^\circ = 7.857 + 0.754 \times 10^{-3}T - 0.773 \times 10^{-5}T^{-2}$
 $H^\circ - H_{2,98}^\circ = 7.857 \times 10^{-3}T + 0.377 \times 10^{-6}T^2 + 0.773 \times 10^{-2}T^{-1} - 2.635$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 2.547 - 3.932 \times 10^{-3}T + 1.843 \times 10^{-6}T^2 - 100.900T^{-1}$
 $\Delta G_f^\circ = 2.547 + 3.932 \times 10^{-3}T \ln T - 1.843 \times 10^{-6}T^2 - 50.450T^{-1} - 46.660 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = 1.432 - 1.669 \times 10^{-3}T + 0.097 \times 10^{-6}T^2 + 54.700T^{-1}$
 $\Delta G_f^\circ = 1.432 + 1.669 \times 10^{-3}T \ln T - 0.097 \times 10^{-6}T^2 + 27.350T^{-1} - 31.477 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -14.726 + 43.071 \times 10^{-3}T - 43.186 \times 10^{-6}T^2 + 1956.900T^{-1}$
 $\Delta G_f^\circ = -14.726 - 43.071 \times 10^{-3}T \ln T + 43.186 \times 10^{-6}T^2 + 978.450T^{-1} + 253.751 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -24.205 + 39.165 \times 10^{-3}T - 23.374 \times 10^{-6}T^2 + 5183.400T^{-1}$
 $\Delta G_f^\circ = -24.205 - 39.165 \times 10^{-3}T \ln T + 23.374 \times 10^{-6}T^2 + 2591.700T^{-1} + 251.904 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH°	ΔG°	
298.15	7.212	53.020	53.020	0	-14.155	-14.532	10.652
300	7.217	53.064	53.021	.013	-14.155	-14.534	10.588
400	7.543	55.185	53.308	.751	-14.171	-14.658	8.009
500	7.846	56.901	53.859	1.521	-14.180	-14.778	6.459
600	8.087	58.354	54.491	2.318	-14.185	-14.897	5.426
700	8.273	59.615	55.134	3.137	-14.185	-15.015	4.688
800	8.414	60.730	55.766	3.971	-14.186	-15.135	4.135
900	8.526	61.727	56.373	4.819	-14.185	-15.253	3.704
1000	8.617	62.631	56.955	5.676	-14.185	-15.372	3.360
1100	8.695	63.456	57.510	6.541	-14.187	-15.492	3.078
1200	8.765	64.215	58.037	7.414	-14.189	-15.609	2.843
1300	8.830	64.919	58.539	8.294	-14.192	-15.727	2.644
1400	8.893	65.576	59.019	9.180	-14.196	-15.846	2.474
1500	8.955	66.192	59.477	10.073	-14.200	-15.964	2.326
1600	9.017	66.772	59.915	10.971	-14.206	-16.082	2.197
1700	9.077	67.320	60.334	11.876	-14.212	-16.198	2.082
1800	9.138	67.841	60.737	12.787	-14.217	-16.314	1.981
1900	9.197	68.336	61.123	13.704	-14.222	-16.430	1.890
2000	9.256	68.810	61.497	14.626	-14.228	-16.548	1.808
2100	9.313	69.263	61.856	15.555	-14.232	-16.663	1.734
2200	9.369	69.697	62.202	16.489	-14.237	-16.778	1.667
2300	9.423	70.115	62.537	17.429	-14.241	-16.894	1.605
2400	9.474	70.517	62.862	18.373	-14.245	-17.010	1.549
2500	9.524	70.905	63.176	19.323	-14.247	-17.125	1.497
2600	9.571	71.279	63.480	20.278	-14.250	-17.240	1.449
2700	9.615	71.641	63.775	21.237	-14.251	-17.355	1.405
2800	9.657	71.992	64.063	22.201	-14.252	-17.469	1.364
2900	9.696	72.331	64.342	23.169	-14.253	-17.582	1.325
3000	9.733	72.660	64.613	24.140	-14.254	-17.698	1.289

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

298.15-2000 K: $C_p^\circ = 7.857 + 0.754 \times 10^{-3}T - 0.773 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 7.857 \times 10^{-3}T + 0.377 \times 10^{-6}T^2 + 0.773 \times 10^{-2}T^3 - 2.635$
 2000-3000 K: $C_p^\circ = 8.917 + 0.318 \times 10^{-3}T - 11.935 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 8.917 \times 10^{-3}T + 0.159 \times 10^{-6}T^2 + 11.935 \times 10^{-2}T^3 - 4.441$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H^\circ = -14.242 + 0.070 \times 10^{-3}T - 0.035 \times 10^{-6}T^2 + 20.550T^{-1}$
 $\Delta G^\circ = -14.242 - 0.070 \times 10^{-3}T \ln T + 0.035 \times 10^{-6}T^2 + 10.275T^{-1} - 0.697 \times 10^{-3}T$
 2000-3000 K: $\Delta H^\circ = -14.355 - 0.008 \times 10^{-3}T + 0.005 \times 10^{-6}T^2 + 248.500T^{-1}$
 $\Delta G^\circ = -14.355 + 0.008 \times 10^{-3}T \ln T - 0.005 \times 10^{-6}T^2 + 124.250T^{-1} = 1.188 \times 10^{-3}T$

Source: Data from Pankratz (91).

SO₂(g)
Sulfur Dioxide (ideal gas)
[Formation: S(c,l) + O₂(g) = SO₂(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° _{2,98})/T	H° - H° _{2,98}	ΔHf°	ΔGf°	
298.15	9.530	59.300	59.300	0.	-70.940	-71.725	52.575
300	9.547	59.359	59.300	.018	-70.945	-71.730	52.254
368.3	10.126	61.377	59.501	.691	-71.139	-71.888	42.658
368.3	10.126	61.377	59.501	.691	-71.235	-71.888	42.658
388.36	10.296	61.918	59.612	.896	-71.293	-71.921	40.473
388.36	10.296	61.918	59.612	.896	-71.706	-71.921	40.473
400	10.395	62.224	59.684	1.016	-71.757	-71.927	39.299
432.02	10.631	63.034	59.903	1.353	-71.915	-71.935	36.390
500	11.132	64.625	60.439	2.093	-72.348	-71.902	31.428
600	11.723	66.709	61.314	3.237	-72.816	-71.766	26.140
700	12.180	68.552	62.219	4.433	-73.198	-71.560	22.342
717.824	12.243	68.859	62.380	4.651	-73.258	-71.517	21.774

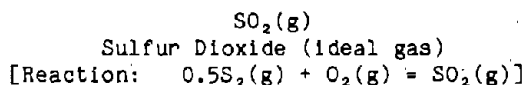
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 11.324 + 1.592x10⁻³T - 2.017x10⁻⁵T²
H° - H°_{2,98} = 11.324x10⁻³T + 0.796x10⁻⁶T² + 2.017x10⁻²T³ = 4.124

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -69.905 - 4.080x10⁻³T + 2.010x10⁻⁶T² + 0.900T⁻¹
ΔGf° = -69.905 + 4.080x10⁻³T ln T - 2.010x10⁻⁶T² + 0.450T⁻¹ - 28.757x10⁻³T
368.3-388.36 K: ΔHf° = -71.020 - 1.817x10⁻³T + 0.264x10⁻⁶T² + 156.500T⁻¹
ΔGf° = -71.020 + 1.817x10⁻³T ln T - 0.264x10⁻⁶T² + 78.250T⁻¹ - 13.574x10⁻³T
388.36-432.02 K: ΔHf° = -87.179 + 42.923x10⁻³T - 43.018x10⁻⁶T² + 2058.700T⁻¹
ΔGf° = -87.179 - 42.923x10⁻³T ln T + 43.018x10⁻⁶T² + 1029.350T⁻¹ + 271.655x10⁻³T
432.02-717.824 K: ΔHf° = -96.657 + 39.017x10⁻³T - 23.206x10⁻⁶T² + 5285.200T⁻¹
ΔGf° = -96.657 - 39.017x10⁻³T ln T + 23.206x10⁻⁶T² + 2642.600T⁻¹ + 269.807x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	9.530	59.300	59.300	0	-86.295	-81.239	59.549
300	9.547	59.359	59.300	.018	-86.297	-81.207	59.158
400	10.395	62.224	59.684	1.016	-86.408	-79.493	43.432
500	11.132	64.625	60.439	2.093	-86.476	-77.755	33.986
600	11.723	66.709	61.314	3.237	-86.511	-76.007	27.685
700	12.180	68.552	62.219	4.433	-86.523	-74.255	23.183
800	12.532	70.202	63.116	5.669	-86.521	-72.503	19.807
900	12.806	71.695	63.987	6.937	-86.507	-70.752	17.181
1000	13.022	73.056	64.827	8.229	-86.485	-69.003	15.080
1100	13.194	74.305	65.632	9.540	-86.461	-67.254	13.362
1200	13.335	75.460	66.405	10.866	-86.434	-65.511	11.931
1300	13.451	76.532	67.143	12.206	-86.404	-63.768	10.720
1400	13.549	77.532	67.849	13.556	-86.377	-62.028	9.683
1500	13.632	78.470	68.527	14.915	-86.350	-60.291	8.784
1600	13.704	79.352	69.176	16.282	-86.325	-58.554	7.998
1700	13.767	80.185	69.799	17.656	-86.303	-56.819	7.304
1800	13.822	80.973	70.398	19.035	-86.284	-55.083	6.688
1900	13.872	81.722	70.975	20.420	-86.268	-53.351	6.137
2000	13.917	82.435	71.530	21.809	-86.257	-51.620	5.641
2100	13.958	83.115	72.066	23.203	-86.249	-49.888	5.192
2200	13.995	83.765	72.583	24.601	-86.244	-48.157	4.784
2300	14.030	84.388	73.083	26.002	-86.245	-46.426	4.411
2400	14.063	84.986	73.566	27.407	-86.249	-44.695	4.070
2500	14.093	85.560	74.034	28.815	-86.256	-42.961	3.756
2600	14.122	86.114	74.489	30.225	-86.269	-41.233	3.466
2700	14.149	86.647	74.929	31.639	-86.283	-39.499	3.197
2800	14.175	87.162	75.357	33.055	-86.303	-37.763	2.948
2900	14.200	87.660	75.772	34.474	-86.325	-36.029	2.715
3000	14.224	88.142	76.177	35.895	-86.352	-34.297	2.499

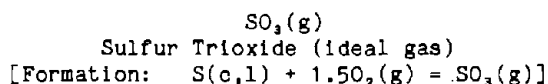
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 11.324 + 1.592 \times 10^{-3}T - 2.017 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 11.324 \times 10^{-3}T + 0.796 \times 10^{-6}T^2 + 2.017 \times 10^2 T^{-1} - 4.124$
 2000-3000 K: $C_p^\circ = 13.942 + 0.138 \times 10^{-3}T - 11.986 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 13.942 \times 10^{-3}T + 0.069 \times 10^{-6}T^2 + 11.986 \times 10^2 T^{-1} - 6.950$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -86.694 - 0.078 \times 10^{-3}T + 0.133 \times 10^{-6}T^2 + 122.350T^{-1}$
 $\Delta G_r^\circ = -86.694 + 0.078 \times 10^{-3}T \ln T - 0.133 \times 10^{-6}T^2 + 61.175T^{-1} + 17.206 \times 10^{-3}T$
 2000-3000 K: $\Delta H_r^\circ = -87.159 + 0.847 \times 10^{-3}T - 0.190 \times 10^{-6}T^2 - 61.400T^{-1}$
 $\Delta G_r^\circ = -87.159 - 0.847 \times 10^{-3}T \ln T + 0.190 \times 10^{-6}T^2 - 30.700T^{-1} + 23.843 \times 10^{-3}T$

Source: Data from Pankratz (91).



T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	12.108	61.344	61.344	0	-94.580	-88.669	64.996
300	12.142	61.419	61.346	.022	-94.588	-88.633	64.568
368.3	13.263	64.029	61.604	.893	-94.824	-87.251	51.774
368.3	13.263	64.029	61.604	.893	-94.920	-87.251	51.774
388.36	13.593	64.742	61.748	1.163	-94.985	-86.831	48.863
388.36	13.593	64.742	61.748	1.163	-95.398	-86.831	48.863
400	13.784	65.146	61.841	1.322	-95.453	-86.573	47.301
432.02	14.200	66.223	62.126	1.770	-95.615	-85.857	43.433
500	15.082	68.367	62.831	2.768	-96.040	-84.284	36.840
600	16.075	71.209	63.996	4.328	-96.469	-81.890	29.828
700	16.824	73.746	65.210	5.975	-96.790	-79.434	24.800
717.824	16.925	74.170	65.427	6.276	-96.837	-78.991	24.049

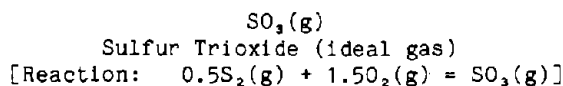
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $C_p^\circ = 16.016 + 2.098 \times 10^{-3}T - 4.029 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 16.016 \times 10^{-3}T + 1.049 \times 10^{-6}T^2 + 4.029 \times 10^{-2}T^{-1} - 6.220$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -94.466 - 3.003 \times 10^{-3}T + 2.012 \times 10^{-6}T^2 + 179.500T^{-1}$
 $\Delta G_f^\circ = -94.466 + 3.003 \times 10^{-3}T \ln T - 2.012 \times 10^{-6}T^2 + 89.750T^{-1} + 1.921 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -95.581 - 0.740 \times 10^{-3}T + 0.265 \times 10^{-6}T^2 + 335.100T^{-1}$
 $\Delta G_f^\circ = -95.581 + 0.740 \times 10^{-3}T \ln T - 0.265 \times 10^{-6}T^2 + 167.550T^{-1} + 17.104 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -111.739 + 44.000 \times 10^{-3}T - 43.016 \times 10^{-6}T^2 + 2237.300T^{-1}$
 $\Delta G_f^\circ = -111.739 - 44.000 \times 10^{-3}T \ln T + 43.016 \times 10^{-6}T^2 + 1118.650T^{-1} + 302.332 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -121.218 + 40.094 \times 10^{-3}T - 23.205 \times 10^{-6}T^2 + 5463.800T^{-1}$
 $\Delta G_f^\circ = -121.218 - 40.094 \times 10^{-3}T \ln T + 23.205 \times 10^{-6}T^2 + 2731.900T^{-1} + 300.485 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15	12.108	61.344	61.344	0	-109.935	-98.183	71.969
300	12.142	61.419	61.346	.022	-109.939	-98.110	71.472
400	13.784	65.146	61.841	1.322	-110.104	-94.139	51.434
500	15.082	68.367	62.831	2.768	-110.168	-90.137	39.399
600	16.075	71.209	63.996	4.328	-110.164	-86.131	31.373
700	16.824	73.746	65.210	5.975	-110.115	-82.129	25.641
800	17.391	76.031	66.422	7.687	-110.035	-78.137	21.346
900	17.823	78.105	67.607	9.448	-109.935	-74.156	18.007
1000	18.157	80.001	68.753	11.248	-109.819	-70.187	15.339
1100	18.419	81.745	69.857	13.077	-109.696	-66.230	13.158
1200	18.628	83.357	70.915	14.930	-109.566	-62.283	11.343
1300	18.796	84.855	71.930	16.802	-109.433	-58.348	9.809
1400	18.933	86.253	72.904	18.688	-109.301	-54.424	8.496
1500	19.046	87.563	73.838	20.587	-109.169	-50.510	7.359
1600	19.140	88.795	74.734	22.497	-109.040	-46.602	6.366
1700	19.219	89.958	75.596	24.415	-108.915	-42.704	5.490
1800	19.286	91.058	76.425	26.340	-108.794	-38.810	4.712
1900	19.344	92.103	77.223	28.272	-108.678	-34.928	4.018
2000	19.393	93.096	77.992	30.209	-108.568	-31.048	3.393
2100	19.436	94.044	78.734	32.150	-108.465	-27.176	2.828
2200	19.474	94.949	79.451	34.096	-108.368	-23.307	2.315
2300	19.507	95.815	80.143	36.045	-108.279	-19.442	1.847
2400	19.536	96.646	80.814	37.997	-108.196	-15.582	1.419
2500	19.562	97.444	81.463	39.952	-108.120	-11.725	1.025
2600	19.585	98.212	82.093	41.909	-108.051	-7.872	.662
2700	19.605	98.951	82.703	43.869	-107.987	-4.019	.325
2800	19.623	99.664	83.296	45.830	-107.932	-.166	.013
2900	19.640	100.353	83.873	47.793	-107.884	3.682	-.278
3000	19.655	101.019	84.433	49.758	-107.842	7.526	-.548

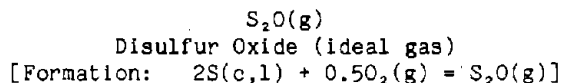
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 16.016 + 2.098 \times 10^{-3}T - 4.029 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 16.016 \times 10^{-3}T + 1.049 \times 10^{-6}T^2 + 4.029 \times 10^{-2}T^{-1} - 6.220$
 2000-3000 K: $C_p^\circ = 18.915 + 0.274 \times 10^{-3}T - 2.782 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 18.915 \times 10^{-3}T + 0.137 \times 10^{-6}T^2 + 2.782 \times 10^{-2}T^{-1} - 8.308$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -111.254 + 1.000 \times 10^{-3}T + 0.134 \times 10^{-6}T^2 + 300.950T^{-1}$
 $\Delta G_r^\circ = -111.254 - 1.000 \times 10^{-3}T \ln T - 0.134 \times 10^{-6}T^2 + 150.475T^{-1} + 47.884 \times 10^{-3}T$
 2000-3000 K: $\Delta H_r^\circ = -110.312 + 1.650 \times 10^{-3}T - 0.227 \times 10^{-6}T^2 - 1296.800T^{-1}$
 $\Delta G_r^\circ = -110.312 - 1.650 \times 10^{-3}T \ln T + 0.227 \times 10^{-6}T^2 - 648.400T^{-1} + 51.835 \times 10^{-3}T$

Source: Data from Pankratz (91).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	10.544	63.796	63.796	0	-9.700	-16.847	12.349
300	10.562	63.861	63.796	.020	-9.706	-16.890	12.305
368.3	11.151	66.092	64.020	.763	-9.973	-18.499	10.977
368.3	11.151	66.092	64.020	.763	-10.165	-18.499	10.977
388.36	11.324	66.688	64.143	.989	-10.249	-18.950	10.664
388.36	11.324	66.688	64.143	.989	-11.075	-18.950	10.664
400	11.424	67.024	64.222	1.121	-11.160	-19.185	10.482
432.02	11.622	67.911	64.463	1.490	-11.433	-19.818	10.025
500	12.041	69.644	65.052	2.296	-12.225	-21.070	9.209
600	12.477	71.880	66.008	3.523	-13.090	-22.754	8.288
700	12.786	73.828	66.989	4.787	-13.814	-24.306	7.589
717.824	12.826	74.150	67.163	5.015	-13.931	-24.571	7.481

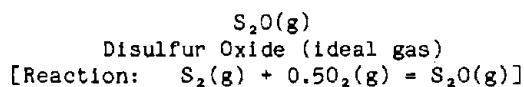
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 12.498 + 0.850x10⁻³T - 1.962x10⁻⁵T⁻²
H° - H°₂₉₈ = 12.498x10⁻³T + 0.425x10⁻⁶T² + 1.962x10⁻²T⁻¹ - 4.422

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -7.333 - 7.465x10⁻³T + 3.608x10⁻⁶T² - 137.600T⁻¹
ΔGf° = -7.333 + 7.465x10⁻³T ln T - 3.608x10⁻⁶T² - 68.800T⁻¹ - 72.592x10⁻³T
368.3-388.36 K: ΔHf° = -9.564 - 2.939x10⁻³T + 0.116x10⁻⁶T² + 173.600T⁻¹
ΔGf° = -9.564 + 2.939x10⁻³T ln T - 0.116x10⁻⁶T² + 86.800T⁻¹ - 42.226x10⁻³T
388.36-432.02 K: ΔHf° = -41.880 + 86.541x10⁻³T - 86.448x10⁻⁶T² + 3978.000T⁻¹
ΔGf° = -41.880 - 86.541x10⁻³T ln T + 86.448x10⁻⁶T² + 1989.000T⁻¹ + 528.231x10⁻³T
432.02-717.824 K: ΔHf° = -60.838 + 78.729x10⁻³T - 46.825x10⁻⁶T² + 10431.000T⁻¹
ΔGf° = -60.838 - 78.729x10⁻³T ln T + 46.825x10⁻⁶T² + 5215.500T⁻¹ + 524.536x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	10.544	63.796	63.796	0	-40.410	-35.874	26.296
300	10.562	63.861	63.796	.020	-40.410	-35.845	26.113
400	11.424	67.024	64.222	1.121	-40.462	-34.316	18.749
500	12.041	69.644	65.052	2.296	-40.480	-32.776	14.326
600	12.477	71.880	66.008	3.523	-40.479	-31.236	11.377
700	12.786	73.828	66.989	4.787	-40.464	-29.696	9.272
800	13.011	75.551	67.954	6.078	-40.444	-28.159	7.693
900	13.177	77.093	68.884	7.388	-40.420	-26.625	6.465
1000	13.303	78.488	69.776	8.712	-40.397	-25.093	5.484
1100	13.399	79.761	70.627	10.047	-40.376	-23.564	4.682
1200	13.475	80.930	71.438	11.391	-40.359	-22.036	4.013
1300	13.536	82.011	72.209	12.742	-40.345	-20.510	3.448
1400	13.585	83.016	72.946	14.098	-40.338	-18.984	2.963
1500	13.625	83.955	73.650	15.458	-40.337	-17.461	2.544
1600	13.658	84.835	74.321	16.822	-40.342	-15.935	2.177
1700	13.686	85.664	74.964	18.190	-40.354	-14.409	1.852
1800	13.709	86.447	75.581	19.559	-40.373	-12.882	1.564
1900	13.729	87.189	76.173	20.931	-40.399	-11.355	1.306
2000	13.747	87.893	76.741	22.305	-40.431	-9.823	1.073

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

298.15-2000 K: $C_p^\circ = 12.498 + 0.850 \times 10^{-3}T - 1.962 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 12.498 \times 10^{-3}T + 0.425 \times 10^{-6}T^2 + 1.962 \times 10^{-2}T^{-1} - 4.422$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -40.911 + 0.540 \times 10^{-3}T - 0.146 \times 10^{-6}T^2 + 105.300T^{-1}$
 $\Delta G_r^\circ = -40.911 - 0.540 \times 10^{-3}T \ln T + 0.146 \times 10^{-6}T^2 + 52.650T^{-1} + 19.334 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mills (80). Other data from JANAF (30).

SO₂Cl₂(g)
Sulfuryl Chloride (ideal gas)
[Formation: S(c,l) + O₂(g) + Cl₂(g) = SO₂Cl₂(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	18.426	74.327	74.327	0	-84.800	-74.177	54.373
300	18.469	74.441	74.328	.034	-84.804	-74.111	53.989
368.3	19.765	78.376	74.722	1.346	-84.923	-71.664	42.525
368.3	19.765	78.376	74.722	1.346	-85.019	-71.664	42.525
388.36	20.146	79.435	74.938	1.746	-85.049	-70.935	39.918
388.36	20.146	79.435	74.938	1.746	-85.462	-70.935	39.918
400	20.367	80.033	75.078	1.982	-85.496	-70.500	38.519
432.02	20.783	81.617	75.505	2.641	-85.603	-69.296	35.055
500	21.667	84.725	76.549	4.088	-85.911	-66.700	29.154
600	22.591	88.762	78.257	6.303	-86.177	-62.831	22.886
700	23.260	92.297	80.014	8.598	-86.338	-58.925	18.397
717.824	23.348	92.883	80.326	9.013	-86.358	-58.227	17.728

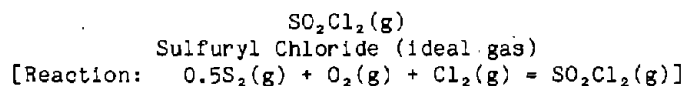
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 22.274 + 2.232x10⁻³T - 4.012x10⁻⁶T⁻²
H° - H₂₉₈° = 22.274x10⁻³T + 1.116x10⁻⁶T² + 4.012x10⁻²T⁻¹ - 8.086

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -84.859 - 1.957x10⁻³T + 2.242x10⁻⁶T² + 132.100T⁻¹
ΔGf° = -84.859 + 1.957x10⁻³TlnT - 2.242x10⁻⁶T² + 66.050T⁻¹ + 24.602x10⁻³T
368.3-388.36 K: ΔHf° = -85.974 + 0.306x10⁻³T + 0.496x10⁻⁶T² + 287.700T⁻¹
ΔGf° = -85.974 - 0.306x10⁻³TlnT - 0.496x10⁻⁶T² + 143.850T⁻¹ + 39.785x10⁻³T
388.36-432.02 K: ΔHf° = -102.132 + 45.046x10⁻³T - 42.786x10⁻⁶T² + 2189.900T⁻¹
ΔGf° = -102.132 - 45.046x10⁻³TlnT + 42.786x10⁻⁶T² + 1094.950T⁻¹ + 325.013x10⁻³T
432.02-717.824 K: ΔHf° = -111.611 + 41.140x10⁻³T - 22.974x10⁻⁶T² + 5416.400T⁻¹
ΔGf° = -111.611 - 41.140x10⁻³TlnT + 22.974x10⁻⁶T² + 2708.200T⁻¹ + 323.166x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/T$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔH°	ΔG°	
298.15	18.426	74.327	74.327	0	-100.155	-83.691	61.346
300	18.469	74.441	74.328	.034	-100.156	-83.588	60.893
400	20.367	80.033	75.078	1.982	-100.147	-78.065	42.652
500	21.667	84.725	76.549	4.088	-100.039	-72.553	31.713
600	22.591	88.762	78.257	6.303	-99.871	-67.072	24.431
700	23.260	92.297	80.014	8.598	-99.663	-61.620	19.239
800	23.754	95.437	81.751	10.949	-99.432	-56.204	15.354
900	24.125	98.257	83.430	13.344	-99.181	-50.814	12.339
1000	24.409	100.815	85.043	15.772	-98.917	-45.455	9.934
1100	24.630	103.152	86.585	18.224	-98.649	-40.122	7.971
1200	24.805	105.303	88.056	20.696	-98.376	-34.813	6.340
1300	24.945	107.294	89.460	23.184	-98.100	-29.528	4.964
1400	25.059	109.147	90.801	25.684	-97.827	-24.264	3.788
1500	25.153	110.879	92.082	28.195	-97.554	-19.019	2.771
1600	25.231	112.505	93.309	30.714	-97.285	-13.792	1.884
1700	25.296	114.036	94.482	33.241	-97.019	-8.579	1.103
1800	25.352	115.484	95.610	35.773	-96.758	-3.385	.411
1900	25.399	116.856	96.692	38.311	-96.501	1.796	-.207
2000	25.440	118.160	97.734	40.853	-96.252	6.963	-.761

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

298.15-2000 K: $\text{Cp}^\circ = 22.274 + 2.232 \times 10^{-3}T - 4.012 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 22.274 \times 10^{-3}T + 1.116 \times 10^{-6}T^2 + 4.012 \times 10^{-2}T^{-1} - 8.086$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta\text{H}^\circ = -101.648 + 2.045 \times 10^{-3}T + 0.365 \times 10^{-6}T^2 + 253.550T^{-1}$
 $\Delta\text{G}^\circ = -101.648 - 2.045 \times 10^{-3}T \ln T - 0.365 \times 10^{-6}T^2 + 126.775T^{-1} + 70.565 \times 10^{-3}T$

Source: Data from Chase (19).

$\text{SOF}_2(\text{g})$
 Thionyl Fluoride (ideal gas)
 [Formation: $\text{S}(\text{c,l}) + 0.5\text{O}_2(\text{g}) + \text{F}_2(\text{g}) = \text{SOF}_2(\text{g})$]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15*	13.648	66.687	66.687	0	-130	-125.850	92.249
300	13.686	66.772	66.689	.025	-130.006	-125.825	91.662
368.3	14.831	69.708	66.980	1.004	-130.173	-124.854	74.088
368.3	14.831	69.708	66.980	1.004	-130.269	-124.854	74.088
388.36	15.167	70.503	67.142	1.305	-130.315	-124.557	70.094
388.36	15.167	70.503	67.142	1.305	-130.728	-124.557	70.094
400	15.362	70.954	67.247	1.483	-130.771	-124.371	67.953
432.02	15.728	72.151	67.566	1.981	-130.907	-123.855	62.655
500	16.506	74.513	68.353	3.080	-131.281	-122.712	53.637
600	17.295	77.596	69.643	4.772	-131.654	-120.962	44.060
700	17.853	80.306	70.976	6.531	-131.932	-119.157	37.202
717.824	17.925	80.756	71.213	6.850	-131.973	-118.830	36.179

*Enthalpy of formation at 298 K estimated.

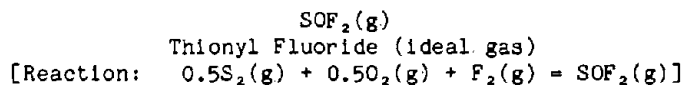
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $C_p^\circ = 17.440 + 1.458 \times 10^{-3}T - 3.757 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 17.440 \times 10^{-3}T + 0.729 \times 10^{-6}T^2 + 3.757 \times 10^{-2}T^3 - 6.525$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -129.653 - 2.857 \times 10^{-3}T + 2.021 \times 10^{-6}T^2 + 97.000T^{-1}$
 $\Delta G_f^\circ = -129.653 + 2.857 \times 10^{-3}T \ln T - 2.021 \times 10^{-6}T^2 + 48.500T^{-1} - 3.465 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -130.768 - 0.594 \times 10^{-3}T + 0.275 \times 10^{-6}T^2 + 252.600T^{-1}$
 $\Delta G_f^\circ = -130.768 + 0.594 \times 10^{-3}T \ln T - 0.275 \times 10^{-6}T^2 + 126.300T^{-1} + 11.718 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -146.927 + 44.146 \times 10^{-3}T - 43.007 \times 10^{-6}T^2 + 2154.800T^{-1}$
 $\Delta G_f^\circ = -146.927 - 44.146 \times 10^{-3}T \ln T + 43.007 \times 10^{-6}T^2 + 1077.400T^{-1} + 296.946 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -156.405 + 40.240 \times 10^{-3}T - 23.196 \times 10^{-6}T^2 + 5381.300T^{-1}$
 $\Delta G_f^\circ = -156.405 - 40.240 \times 10^{-3}T \ln T + 23.196 \times 10^{-6}T^2 + 2690.650T^{-1} + 295.099 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔH°	ΔG°	
298.15*	13.648	66.687	66.687	0	-145.355	-135.364	99.223
300	13.686	66.772	66.689	.025	-145.358	-135.302	98.566
400	15.362	70.954	67.247	1.483	-145.423	-131.937	72.086
500	16.506	74.513	68.353	3.080	-145.408	-128.565	56.195
600	17.295	77.596	69.643	4.772	-145.348	-125.203	45.604
700	17.853	80.306	70.976	6.531	-145.257	-121.852	38.043
800	18.255	82.718	72.296	8.338	-145.146	-118.516	32.377
900	18.553	84.886	73.576	10.179	-145.023	-115.194	27.973
1000	18.778	86.853	74.807	12.046	-144.893	-111.887	24.453
1100	18.951	88.651	75.985	13.933	-144.759	-108.592	21.575
1200	19.087	90.306	77.110	15.835	-144.623	-105.310	19.179
1300	19.196	91.839	78.186	17.749	-144.486	-102.041	17.154
1400	19.284	93.264	79.211	19.674	-144.352	-98.780	15.420
1500	19.356	94.597	80.193	21.606	-144.220	-95.530	13.919
1600	19.416	95.849	81.134	23.544	-144.092	-92.290	12.606
1700	19.466	97.027	82.033	25.489	-143.965	-89.053	11.448
1800	19.508	98.141	82.898	27.437	-143.846	-85.827	10.421
1900	19.544	99.197	83.729	29.390	-143.728	-82.607	9.502
2000	19.575	100.200	84.527	31.346	-143.617	-79.393	8.676

*Enthalpy of formation at 298 K estimated.

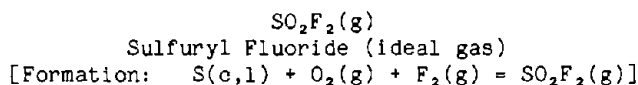
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $\text{Cp}^\circ = 17.440 + 1.458 \times 10^{-3}T - 3.757 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 17.440 \times 10^{-3}T + 0.729 \times 10^{-6}T^2 + 3.757 \times 10^{-2}T^3 - 6.525$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta\text{H}^\circ = -146.442 + 1.145 \times 10^{-3}T + 0.144 \times 10^{-6}T^2 + 218.450T^{-1}$
 $\Delta\text{G}^\circ = -146.442 - 1.145 \times 10^{-3}T \ln T - 0.144 \times 10^{-6}T^2 + 109.225T^{-1} + 42.498 \times 10^{-3}T$

Source: Data from Chase (19) who estimated enthalpy of formation at 298 K.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHf°	ΔGf°	
298.15	15.732	67.761	67.761	0	-181.300	-170.165	124.732
300	15.787	67.858	67.761	.029	-181.308	-170.095	123.913
368.3	17.494	71.285	68.100	1.173	-181.552	-167.515	99.402
368.3	17.494	71.285	68.100	1.173	-181.648	-167.515	99.402
388.36	17.996	72.226	68.290	1.529	-181.711	-166.743	93.833
388.36	17.996	72.226	68.290	1.529	-182.124	-166.743	93.833
400	18.287	72.762	68.412	1.740	-182.176	-166.281	90.851
432.02	18.858	74.192	68.788	2.335	-182.330	-165.003	83.471
500	20.070	77.046	69.720	3.663	-182.725	-162.243	70.915
600	21.349	80.824	71.262	5.737	-183.093	-158.109	57.590
700	22.276	84.189	72.873	7.921	-183.335	-153.924	48.057
717.824	22.398	84.751	73.161	8.319	-183.367	-153.175	46.636

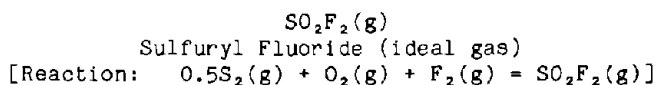
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta\text{H}^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta\text{H}^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta\text{H}^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $\text{Cp}^\circ = 21.424 + 2.574 \times 10^{-3}T - 5.742 \times 10^{-5}T^{-2}$
 $\text{H}^\circ - \text{H}_{298}^\circ = 21.424 \times 10^{-3}T + 1.287 \times 10^{-6}T^2 + 5.742 \times 10^{-2}T^{-1} - 8.428$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta\text{Hf}^\circ = -181.680 - 2.488 \times 10^{-3}T + 2.327 \times 10^{-6}T^2 + 272.900T^{-1}$
 $\Delta\text{Gf}^\circ = -181.680 + 2.488 \times 10^{-3}T \ln T - 2.327 \times 10^{-6}T^2 + 136.450T^{-1} + 23.607 \times 10^{-3}T$
 368.3-388.36 K: $\Delta\text{Hf}^\circ = -182.795 - 0.225 \times 10^{-3}T + 0.581 \times 10^{-6}T^2 + 428.500T^{-1}$
 $\Delta\text{Gf}^\circ = -182.795 + 0.225 \times 10^{-3}T \ln T - 0.581 \times 10^{-6}T^2 + 214.250T^{-1} + 38.790 \times 10^{-3}T$
 388.36-432.02 K: $\Delta\text{Hf}^\circ = -198.954 + 44.515 \times 10^{-3}T - 42.701 \times 10^{-6}T^2 + 2330.700T^{-1}$
 $\Delta\text{Gf}^\circ = -198.954 - 44.515 \times 10^{-3}T \ln T + 42.701 \times 10^{-6}T^2 + 1165.350T^{-1} + 324.018 \times 10^{-3}T$
 432.02-717.824 K: $\Delta\text{Hf}^\circ = -208.432 + 40.609 \times 10^{-3}T - 22.889 \times 10^{-6}T^2 + 5557.200T^{-1}$
 $\Delta\text{Gf}^\circ = -208.432 - 40.609 \times 10^{-3}T \ln T + 22.889 \times 10^{-6}T^2 + 2778.600T^{-1} + 322.171 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15	15.732	67.761	67.761	0	-196.655	-179.678	131.706
300	15.787	67.858	67.761	.029	-196.660	-179.573	130.817
400	18.287	72.762	68.412	1.740	-196.827	-173.847	94.984
500	20.070	77.046	69.720	3.663	-196.853	-168.096	73.474
600	21.349	80.824	71.262	5.737	-196.788	-162.350	59.135
700	22.276	84.189	72.873	7.921	-196.660	-156.620	48.898
800	22.960	87.210	74.480	10.184	-196.492	-150.912	41.227
900	23.474	89.946	76.049	12.507	-196.294	-145.226	35.265
1000	23.866	92.440	77.583	14.857	-196.077	-139.564	30.501
1100	24.172	94.730	79.023	17.278	-195.846	-133.922	26.608
1200	24.413	96.844	80.422	19.707	-195.607	-128.304	23.367
1300	24.607	98.806	81.761	22.159	-195.361	-122.704	20.628
1400	24.764	100.635	83.044	24.627	-195.116	-117.126	18.284
1500	24.894	102.348	84.274	27.111	-194.867	-111.563	16.255
1600	25.002	103.958	85.454	29.606	-194.620	-106.017	14.481
1700	25.092	105.477	86.589	32.110	-194.376	-100.487	12.918
1800	25.169	106.913	87.678	34.623	-194.135	-94.970	11.531
1900	25.234	108.276	88.727	37.144	-193.896	-89.467	10.291
2000	25.291	109.572	89.737	39.670	-193.665	-83.978	9.177

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

298.15-2000 K: $C_p^\circ = 21.424 + 2.574 \times 10^{-3}T - 5.742 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 21.424 \times 10^{-3}T + 1.287 \times 10^{-6}T^2 + 5.742 \times 10^{-2}T^{-1} - 8.428$

Reaction equations (kcal/mol):

298.15-2000 K: $\Delta H_r^\circ = -198.469 + 1.514 \times 10^{-3}T + 0.450 \times 10^{-5}T^2 + 394.350T^{-1}$
 $\Delta G_r^\circ = -198.469 - 1.514 \times 10^{-3}T \ln T - 0.450 \times 10^{-6}T^2 + 197.175T^{-1} + 69.570 \times 10^{-3}T$

Source: Data from Chase (19).

SbS(g)
Antimony Monosulfide (ideal gas)
[Formation: Sb(c) + S(c,l) = SbS(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	8.285	59.656	59.656	0	44.400	32.142	-23.560
300	8.292	59.708	59.658	.015	44.394	32.066	-23.360
368.3	8.483	61.431	59.830	.590	44.168	29.284	-17.377
368.3	8.483	61.431	59.830	.590	44.072	29.284	-17.377
388.36	8.539	61.882	59.924	.760	44.000	28.481	-16.027
388.36	8.539	61.882	59.924	.760	43.587	28.481	-16.027
400	8.572	62.135	59.985	.860	43.527	28.029	-15.314
432.02	8.637	62.798	60.169	1.136	43.340	26.795	-13.555
500	8.774	64.070	60.616	1.727	42.830	24.234	-10.592
600	8.962	65.686	61.329	2.614	42.220	20.570	-7.492
700	9.148	67.082	62.053	3.520	41.667	17.009	-5.310
717.824	9.179	67.312	62.181	3.683	41.573	16.383	-4.988

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-3000 K: Cp° = 9.209 + 0.338x10⁻³T - 0.911x10⁻⁵T²
H°- H₂₉₈° = 9.209x10⁻³T + 0.169x10⁻⁶T² + 0.911x10⁻²T³ - 3.066

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 45.689 - 4.053x10⁻³T + 0.714x10⁻⁶T² - 42.900T⁻¹
ΔGf° = 45.689 + 4.053x10⁻³TlnT - 0.714x10⁻⁶T² - 21.450T⁻¹ - 68.076x10⁻³T
368.3-388.36 K: ΔHf° = 44.574 - 1.790x10⁻³T - 1.032x10⁻⁶T² + 112.700T⁻¹
ΔGf° = 44.574 + 1.790x10⁻³TlnT + 1.032x10⁻⁶T² + 56.350T⁻¹ - 52.893x10⁻³T
388.36-432.02 K: ΔHf° = 28.415 + 42.950x10⁻³T - 44.314x10⁻⁶T² + 2014.900T⁻¹
ΔGf° = 28.415 - 42.950x10⁻³TlnT + 44.314x10⁻⁶T² + 1007.450T⁻¹ + 232.335x10⁻³T
432.02-717.824 K: ΔHf° = 18.937 + 39.044x10⁻³T - 24.502x10⁻⁶T² + 5241.400T⁻¹
ΔGf° = 18.937 - 39.044x10⁻³TlnT + 24.502x10⁻⁶T² + 2620.700T⁻¹ + 230.488x10⁻³T

SbS(g)
Antimony Monosulfide (ideal gas)
[Reaction: $\text{Sb(c,l)} + 0.5\text{S}_2(\text{g}) = \text{SbS(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	8.285	59.656	59.656	0	29.045	22.628	-16.586
300	8.292	59.708	59.658	.015	29.042	22.589	-16.456
400	8.572	62.135	59.985	.860	28.876	20.463	-11.180
500	8.774	64.070	60.616	1.727	28.703	18.380	-8.034
600	8.962	65.686	61.329	2.614	28.526	16.329	-5.948
700	9.148	67.082	62.053	3.520	28.342	14.314	-4.469
800	9.323	68.315	62.761	4.443	28.144	12.318	-3.365
900	9.479	69.422	63.440	5.384	27.925	10.356	-2.515
903.9	9.484	69.463	63.466	5.421	27.915	10.280	-2.486
903.9	9.484	69.463	63.466	5.421	23.165	10.280	-2.486
1000	9.608	70.428	64.090	6.338	22.936	8.917	-1.949
1100	9.710	71.349	64.709	7.304	22.705	7.531	-1.496
1200	9.787	72.197	65.298	8.279	22.479	6.159	-1.122
1300	9.840	72.982	65.858	9.261	22.256	4.809	-.808
1400	9.874	73.713	66.394	10.247	22.034	3.481	-.543
1500	9.892	74.395	66.905	11.235	21.810	2.166	-.316
1600	9.898	75.034	67.393	12.225	21.584	.858	-.117
1700	9.895	75.634	67.861	13.214	21.354	-.440	.057
1800	9.886	76.199	68.308	14.203	21.120	-1.712	.208
1860	9.878	76.523	68.568	14.796	20.979	-2.463	.289

Phase changes: 903.9 K, melting point of Sb; ΔH° = 4.750 kcal/mol.

1860 K, boiling point of Sb to equilibrium mixture of Sb(g), Sb₂(g), and Sb₃(g).

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

298.15-3000 K: $\text{Cp}^\circ = 9.209 + 0.338 \times 10^{-3}T - 0.911 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 9.209 \times 10^{-3}T + 0.169 \times 10^{-6}T^2 + 0.911 \times 10^{-2}T^{-1} - 3.066$

Reaction equations (kcal/mol):

298.15-903.9 K: $\Delta\text{Hr}^\circ = 28.900 - 0.051 \times 10^{-3}T - 1.163 \times 10^{-6}T^2 + 78.550T^{-1}$
 $\Delta\text{Gr}^\circ = 28.900 + 0.051 \times 10^{-3}T \ln T + 1.163 \times 10^{-6}T^2 + 39.275T^{-1} - 22.113 \times 10^{-3}T$
 903.9-1860 K: $\Delta\text{Hr}^\circ = 25.397 - 2.463 \times 10^{-3}T + 0.009 \times 10^{-6}T^2 + 56.950T^{-1}$
 $\Delta\text{Gr}^\circ = 25.397 + 2.463 \times 10^{-3}T \ln T - 0.009 \times 10^{-6}T^2 + 28.475T^{-1} - 33.582 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Prusaczyk (101). Other data based on Prusaczyk (101) and Shimauchi (107).

(SbS)₂(g)
Dimeric Antimony Monosulfide (ideal gas)
[Formation: 2Sb(c) + 2S(c,l) = (SbS)₂(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	17.130	81.283	81.283	0	40.700	27.521	-20.174
300	17.155	81.389	81.283	.032	40.690	27.442	-19.991
368.3	17.830	84.990	81.645	1.232	40.289	24.468	-14.519
368.3	17.830	84.990	81.645	1.232	40.097	24.468	-14.519
388.36	18.029	85.941	81.843	1.591	39.972	23.621	-13.293
388.36	18.029	85.941	81.843	1.591	39.146	23.621	-13.293
400	18.144	86.475	81.970	1.802	39.036	23.157	-12.652
432.02	18.320	87.879	82.357	2.386	38.695	21.898	-11.078
500	18.695	90.588	83.296	3.646	37.752	19.335	-8.451
600	19.025	94.028	84.805	5.534	36.646	15.752	-5.737
700	19.235	96.978	86.339	7.447	35.641	12.355	-3.857
717.824	19.260	97.462	86.610	7.790	35.470	11.765	-3.582

*Data except enthalpy of formation at 298 K estimated.

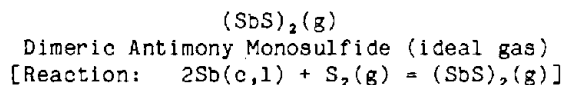
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-3000 K: Cp° = 19.584 + 0.134x10⁻³T - 2.216x10⁻⁵T⁻²
H° - H°₂₉₈ = 19.584x10⁻³T + 0.067x10⁻⁶T² + 2.216x10⁻²T⁻¹ - 6.588

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 42.822 - 6.940x10⁻³T + 1.157x10⁻⁶T² - 46.400T⁻¹
ΔGf° = 42.822 + 6.940x10⁻³T lnT - 1.157x10⁻⁶T² - 23.200T⁻¹ - 90.253x10⁻³T
368.3-388.36 K: ΔHf° = 40.592 - 2.414x10⁻³T - 2.335x10⁻⁶T² + 264.800T⁻¹
ΔGf° = 40.592 + 2.414x10⁻³T lnT + 2.335x10⁻⁶T² + 132.400T⁻¹ - 59.887x10⁻³T
388.36-432.02 K: ΔHf° = 8.275 + 87.066x10⁻³T - 88.899x10⁻⁶T² + 4069.200T⁻¹
ΔGf° = 8.275 - 87.066x10⁻³T lnT + 88.899x10⁻⁶T² + 2034.600T⁻¹ + 510.569x10⁻³T
432.02-717.824 K: ΔHf° = -10.682 + 79.254x10⁻³T - 49.275x10⁻⁶T² + 10522.200T⁻¹
ΔGf° = -10.682 - 79.254x10⁻³T lnT + 49.275x10⁻⁶T² + 5261.100T⁻¹ + 506.874x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHr°	ΔGr°	
298.15*	17.130	81.283	81.283	0	9.990	8.494	-6.226
300	17.155	81.389	81.283	.032	9.986	8.488	-6.183
400	18.144	86.475	81.970	1.802	9.734	8.026	-4.385
500	18.695	90.588	83.296	3.646	9.497	7.629	-3.334
600	19.025	94.028	84.805	5.534	9.257	7.270	-2.648
700	19.235	96.978	86.339	7.447	8.991	6.965	-2.174
800	19.377	99.556	87.834	9.378	8.679	6.688	-1.827
900	19.477	101.844	89.265	11.321	8.302	6.464	-1.570
903.9	19.480	101.928	89.320	11.397	8.286	6.456	-1.561
903.9	19.480	101.928	89.320	11.397	-1.214	6.456	-1.561
1000	19.550	103.900	90.627	13.273	-1.631	7.286	-1.592
1100	19.604	105.766	91.920	15.231	-2.068	8.210	-1.631
1200	19.646	107.474	93.146	17.193	-2.508	9.157	-1.668
1300	19.679	109.048	94.310	19.159	-2.951	10.145	-1.706
1400	19.705	110.507	95.415	21.129	-3.398	11.183	-1.746
1500	19.726	111.867	96.467	23.100	-3.851	12.247	-1.784
1600	19.744	113.141	97.470	25.074	-4.308	13.322	-1.820
1700	19.758	114.338	98.427	27.049	-4.772	14.423	-1.854
1800	19.770	115.468	99.343	29.025	-5.240	15.570	-1.890
1860	19.777	116.116	99.873	30.212	-5.523	16.284	-1.913

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 903.9 K, melting point of Sb; $\Delta\text{H}^\circ = 4.750$ kcal/mol.

1860 K, boiling point of Sb to equilibrium mixture of Sb(g), Sb₂(g), and Sb₃(g).

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

298.15-3000 K: $\text{Cp}^\circ = 19.584 + 0.134 \times 10^{-3}T - 2.216 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 19.584 \times 10^{-3}T + 0.067 \times 10^{-6}T^2 + 2.216 \times 10^{-2}T^{-1} - 6.588$

Reaction equations (kcal/mol):

298.15-903.9 K: $\Delta\text{Hr}^\circ = 9.244 + 1.065 \times 10^{-3}T - 2.597 \times 10^{-6}T^2 + 196.500T^{-1}$
 $\Delta\text{Gr}^\circ = 9.244 - 1.065 \times 10^{-3}T \ln T + 2.597 \times 10^{-6}T^2 + 98.250T^{-1} + 1.673 \times 10^{-3}T$
 903.9-1860 K: $\Delta\text{Hr}^\circ = 2.237 - 3.759 \times 10^{-3}T - 0.253 \times 10^{-6}T^2 + 153.300T^{-1}$
 $\Delta\text{Gr}^\circ = 2.237 + 3.759 \times 10^{-3}T \ln T + 0.253 \times 10^{-6}T^2 + 76.650T^{-1} - 21.266 \times 10^{-3}T$

Source: Data based on Prusaczyk (101) who estimated molecular constants.

(SbS)₃(g)
 Trimeric Antimony Monosulfide (ideal gas)
 [Formation: 3Sb(c) + 3S(c,l) = (SbS)₃(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	27.247	92.047	92.047	0	32.900	22.040	-16.156
300	27.293	92.216	92.049	.050	32.887	21.976	-16.009
368.3	28.496	97.962	92.625	1.966	32.402	19.543	-11.597
368.3	28.496	97.962	92.625	1.966	32.114	19.543	-11.597
388.36	28.850	99.483	92.940	2.541	31.961	18.865	-10.616
388.36	28.850	99.483	92.940	2.541	30.722	18.865	-10.616
400	29.055	100.338	93.143	2.878	30.579	18.511	-10.114
432.02	29.349	102.587	93.761	3.813	30.127	17.560	-8.883
500	29.973	106.930	95.262	5.834	28.843	15.694	-6.860
600	30.502	112.446	97.679	8.860	27.378	13.194	-4.806
700	30.833	117.175	100.135	11.928	26.069	10.944	-3.417
717.824	30.872	117.951	100.568	12.478	25.848	10.563	-3.216

*Data except enthalpy of formation at 298 K estimated.

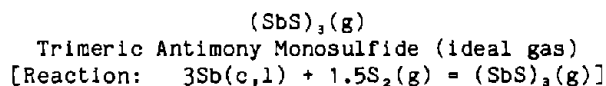
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-3000 K: Cp° = 31.478 + 0.154x10⁻³T - 3.802x10⁻⁵T⁻²
 H° - H°₂₉₈ = 31.478x10⁻³T + 0.077x10⁻⁶T² + 3.802x10⁻²T⁻¹ - 10.667

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 35.298 - 8.308x10⁻³T + 1.712x10⁻⁶T² - 21.800T⁻¹
 ΔGf° = 35.298 + 8.308x10⁻³TlnT - 1.712x10⁻⁶T² - 10.900T⁻¹ - 91.169x10⁻³T
 368.3-388.36 K: ΔHf° = 31.953 - 1.519x10⁻³T - 3.526x10⁻⁶T² + 445.000T⁻¹
 ΔGf° = 31.953 + 1.519x10⁻³TlnT + 3.526x10⁻⁶T² + 222.500T⁻¹ - 45.621x10⁻³T
 388.36-432.02 K: ΔHf° = -16.522 + 132.701x10⁻³T - 133.372x10⁻⁶T² + 6151.600T⁻¹
 ΔGf° = -16.522 - 132.701x10⁻³TlnT + 133.372x10⁻⁶T² + 3075.800T⁻¹ + 810.065x10⁻³T
 432.02-717.824 K: ΔHf° = -44.958 + 120.983x10⁻³T - 73.936x10⁻⁶T² + 15831.100T⁻¹
 ΔGf° = -44.958 - 120.983x10⁻³TlnT + 73.936x10⁻⁶T² + 7915.550T⁻¹ + 804.522x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHr°	ΔGr°	
298.15*	27.247	92.047	92.047	0	-13.165	-6.501	4.765
300	27.293	92.216	92.049	.050	-13.169	-6.456	4.703
400	29.055	100.338	93.143	2.878	-13.374	-4.186	2.287
500	29.973	106.930	95.262	5.834	-13.539	-1.866	.816
600	30.502	112.446	97.679	8.860	-13.705	.471	-.172
700	30.833	117.175	100.135	11.928	-13.906	2.859	-.892
800	31.052	121.307	102.528	15.023	-14.176	5.259	-1.437
900	31.205	124.974	104.823	18.136	-14.542	7.714	-1.873
903.9	31.209	125.109	104.910	18.258	-14.559	7.811	-1.889
903.9	31.209	125.109	104.910	18.258	-28.809	7.811	-1.889
1000	31.315	128.267	107.005	21.262	-29.244	11.715	-2.560
1100	31.397	131.256	109.076	24.398	-29.701	15.849	-3.149
1200	31.460	133.991	111.040	27.541	-30.161	20.001	-3.643
1300	31.509	136.511	112.903	30.690	-30.625	24.199	-4.068
1400	31.548	138.847	114.674	33.842	-31.099	28.452	-4.441
1500	31.579	141.025	116.359	36.999	-31.578	32.733	-4.769
1600	31.605	143.064	117.965	40.158	-32.065	37.017	-5.056
1700	31.627	144.981	119.499	43.320	-32.562	41.325	-5.313
1800	31.645	146.789	120.965	46.483	-33.065	45.694	-5.548
1860	31.654	147.826	121.814	48.383	-33.370	48.348	-5.681

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 903.9 K, melting point of Sb; $\Delta\text{H}^\circ = 4.750$ kcal/mol.

1860 K, boiling point of Sb to equilibrium mixture of $\text{Sb}(\text{g})$, $\text{Sb}_2(\text{g})$, and $\text{Sb}_3(\text{g})$.

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

298.15-3000 K: $\text{Cp}^\circ = 31.478 + 0.154 \times 10^{-3}T - 3.802 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 31.478 \times 10^{-3}T + 0.077 \times 10^{-6}T^2 + 3.802 \times 10^{-2}T^{-1} - 10.667$

Reaction equations (kcal/mol):

298.15-903.9 K: $\Delta\text{Hr}^\circ = -15.069 + 3.699 \times 10^{-3}T - 3.919 \times 10^{-6}T^2 + 342.550T^{-1}$
 $\Delta\text{Gr}^\circ = -15.069 - 3.699 \times 10^{-3}T \ln T + 3.919 \times 10^{-6}T^2 + 171.275T^{-1} + 46.720 \times 10^{-3}T$
 903.9-1860 K: $\Delta\text{Hr}^\circ = -25.579 - 3.537 \times 10^{-3}T - 0.403 \times 10^{-6}T^2 + 277.750T^{-1}$
 $\Delta\text{Gr}^\circ = -25.579 + 3.537 \times 10^{-3}T \ln T + 0.403 \times 10^{-6}T^2 + 138.875T^{-1} + 12.312 \times 10^{-3}T$

Source: Data based on Prusaczyk (101) who estimated molecular constants.

(SbS)₄(g)
Tetrameric Antimony Monosulfide (ideal gas)
[Formation: 4Sb(c) + 4S(c,1) = (SbS)₄(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	40.873	123.176	123.176	0	29.400	14.787	-10.839
300	40.905	123.429	123.176	.076	29.392	14.701	-10.710
368.3	41.703	131.920	124.035	2.904	29.019	11.394	-6.761
368.3	41.703	131.920	124.035	2.904	28.635	11.394	-6.761
388.36	41.938	134.138	124.500	3.743	28.503	10.461	-5.887
388.36	41.938	134.138	124.500	3.743	26.851	10.461	-5.887
400	42.074	135.379	124.799	4.232	26.700	9.971	-5.448
432.02	42.257	138.626	125.705	5.582	26.201	8.648	-4.375
500	42.647	144.836	127.894	8.471	24.683	6.019	-2.631
600	42.967	152.642	131.387	12.753	22.977	2.437	-.888
700	43.163	159.281	134.908	17.061	21.449	-.851	.266
717.824	43.186	160.366	135.527	17.830	21.190	-1.413	.430

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-3000 K: Cp° = 43.627 + 0.044x10⁻³T - 2.460x10⁻⁵T⁻²
H° - H°₂₉₈ = 43.627x10⁻³T + 0.022x10⁻⁶T² + 2.460x10⁻²T⁻¹ - 13.834

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 32.986 - 9.421x10⁻³T + 2.202x10⁻⁶T² - 290 T⁻¹
ΔGf° = 32.986 + 9.421x10⁻³TlnT - 2.202x10⁻⁶T² - 145.000T⁻¹ - 112.428x10⁻³T
368.3-388.36 K: ΔHf° = 28.525 - 0.369x10⁻³T - 4.782x10⁻⁶T² + 332.400T⁻¹
ΔGf° = 28.525 + 0.369x10⁻³TlnT + 4.782x10⁻⁶T² + 166.200T⁻¹ - 51.696x10⁻³T
388.36-432.02 K: ΔHf° = -36.108 + 178.591x10⁻³T - 177.910x10⁻⁶T² + 7941.200T⁻¹
ΔGf° = -36.108 + 178.591x10⁻³TlnT + 177.910x10⁻⁶T² + 3970.600T⁻¹ + 1089.217x10⁻³T
432.02-717.824 K: ΔHf° = -74.023 + 162.967x10⁻³T - 98.662x10⁻⁶T² + 20847.200T⁻¹
ΔGf° = -74.023 - 162.967x10⁻³TlnT + 98.662x10⁻⁶T² + 10423.600T⁻¹ + 1081.827x10⁻³T

(SbS)₄(g)
 Tetrameric Antimony Monosulfide (ideal gas)
 [Reaction: 4Sb(c,l) + 2S₂(g) = (SbS)₄(g)]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15*	40.873	123.176	123.176	0	-32.020	-23.268	17.055
300	40.905	123.429	123.176	.076	-32.016	-23.208	16.907
400	42.074	135.379	124.799	4.232	-31.904	-20.292	11.087
500	42.647	144.836	127.894	8.471	-31.827	-17.394	7.603
600	42.967	152.642	131.387	12.753	-31.801	-14.527	5.291
700	43.163	159.281	134.908	17.061	-31.851	-11.631	3.631
800	43.291	165.054	138.324	21.384	-32.014	-8.750	2.390
900	43.380	170.158	141.582	25.718	-32.320	-5.819	1.413
903.9	43.382	170.346	141.706	25.887	-32.336	-5.702	1.379
903.9	43.382	170.346	141.706	25.887	-51.336	-5.702	1.379
1000	43.444	174.732	144.673	30.059	-51.749	- .847	.185
1100	43.491	178.875	147.597	34.406	-52.192	4.288	-.852
1200	43.527	182.661	150.363	38.757	-52.645	9.430	-1.717
1300	43.555	186.146	152.984	43.111	-53.109	14.618	-2.458
1400	43.578	189.375	155.469	47.468	-53.586	19.871	-3.102
1500	43.596	192.382	157.831	51.826	-54.076	25.148	-3.664
1600	43.610	195.196	160.079	56.187	-54.577	30.421	-4.155
1700	43.623	197.840	162.224	60.548	-55.094	35.717	-4.592
1800	43.633	200.334	164.272	64.911	-55.619	41.084	-4.988
1860	43.638	201.764	165.458	67.529	-55.940	44.344	-5.210

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 903.9 K, melting point of Sb; ΔH° = 4.750 kcal/mol.

1860 K, boiling point of Sb to equilibrium mixture of Sb(g), Sb₂(g), and Sb₄(g).

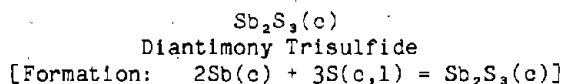
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

$$298.15-3000 \text{ K: } \begin{aligned} \text{Cp}^\circ &= 43.627 + 0.044 \times 10^{-3} T - 2.460 \times 10^{-5} T^2 \\ \text{H}^\circ - \text{H}^\circ_{298} &= 43.627 \times 10^{-3} T + 0.022 \times 10^{-6} T^2 + 2.460 \times 10^{-2} T^{-1} - 13.834 \end{aligned}$$

Reaction equations (kcal/mol):

$$\begin{aligned} 298.15-903.9 \text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= -34.170 + 6.589 \times 10^{-3} T - 5.306 \times 10^{-6} T^2 + 195.800 T^{-1} \\ \Delta \text{Gr}^\circ &= -34.170 - 6.589 \times 10^{-3} T \ln T + 5.306 \times 10^{-6} T^2 + 97.900 T^{-1} + 71.424 \times 10^{-3} T \end{aligned} \\ 903.9-1860 \text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= -48.183 - 3.059 \times 10^{-3} T - 0.618 \times 10^{-6} T^2 + 109.400 T^{-1} \\ \Delta \text{Gr}^\circ &= -48.183 + 3.059 \times 10^{-3} T \ln T + 0.618 \times 10^{-6} T^2 + 54.700 T^{-1} + 25.547 \times 10^{-3} T \end{aligned} \end{aligned}$$

Source: Data based on Prusaczyk (101) who estimated molecular constants.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	28.650	43.540	43.540	0	-33.890	-33.531	24.579
300	28.669	43.717	43.540	.053	-33.889	-33.527	24.424
350	29.163	48.174	43.891	1.499	-33.888	-33.467	20.898
368.3	29.330	49.665	44.141	2.034	-33.892	-33.445	19.846
368.3	29.330	49.665	44.141	2.034	-34.180	-33.445	19.846
388.36	29.514	51.226	44.467	2.625	-34.194	-33.403	18.797
388.36	29.514	51.226	44.467	2.625	-35.433	-33.403	18.797
400	29.620	52.099	44.676	2.969	-35.497	-33.342	18.217
432.02	29.906	54.389	45.311	3.922	-35.732	-33.162	16.776
450	30.067	55.612	45.699	4.461	-36.085	-33.046	16.049
500	30.511	58.803	46.853	5.975	-36.556	-32.682	14.285
550	30.958	61.733	48.075	7.512	-36.963	-32.280	12.827
600	31.415	64.446	49.328	9.071	-37.311	-31.839	11.597
650	31.883	66.979	50.588	10.654	-37.596	-31.364	10.546
700	32.366	69.360	51.846	12.260	-37.840	-30.876	9.640
717.824	32.542	70.176	52.291	12.838	-37.913	-30.697	9.346

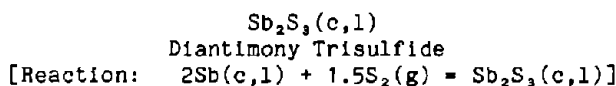
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-823 K: Cp° = 25.971 + 9.160x10⁻³T - 0.046x10⁻⁵T⁻²
 H°- H₂₉₈° = 25.971x10⁻³T + 4.580x10⁻⁶T² + 0.046x10⁻²T⁻¹ - 8.166

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -30.539 - 8.727x10⁻³T + 7.387x10⁻⁶T² - 419.000T⁻¹
 ΔGf° = -30.539 + 8.727x10⁻³TlnT - 7.387x10⁻⁶T² - 209.500T⁻¹ - 55.199x10⁻³T
 368.3-388.36 K: ΔHf° = -33.885 - 1.938x10⁻³T + 2.149x10⁻⁶T² + 47.800T⁻¹
 ΔGf° = -33.885 + 1.938x10⁻³TlnT - 2.149x10⁻⁶T² + 23.900T⁻¹ - 9.650x10⁻³T
 388.36-432.02 K: ΔHf° = -82.360 + 132.282x10⁻³T - 127.697x10⁻⁶T² + 5754.400T⁻¹
 ΔGf° = -82.360 - 132.282x10⁻³TlnT + 127.697x10⁻⁶T² + 2877.200T⁻¹ + 846.035x10⁻³T
 432.02-717.824 K: ΔHf° = -110.796 + 120.564x10⁻³T - 68.261x10⁻⁶T² + 15433.900T⁻¹
 ΔGf° = -110.796 - 120.564x10⁻³TlnT + 68.261x10⁻⁶T² + 7716.950T⁻¹ + 840.493x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHr°	ΔGr°	
298.15	28.650	43.540	43.540	0	-79.955	-62.072	45.500
300	28.669	43.717	43.540	.053	-79.945	-61.958	45.136
350	29.163	48.174	43.891	1.499	-79.700	-58.982	36.829
400	29.620	52.099	44.676	2.969	-79.450	-56.039	30.618
450	30.067	55.612	45.699	4.461	-79.198	-53.125	25.800
500	30.511	58.803	46.853	5.975	-78.938	-50.242	21.960
550	30.958	61.733	48.075	7.512	-78.671	-47.393	18.832
600	31.415	64.446	49.328	9.071	-78.395	-44.562	16.231
650	31.883	66.979	50.588	10.654	-78.108	-41.747	14.037
700	32.366	69.360	51.846	12.260	-77.815	-38.962	12.164
750	32.861	71.609	53.088	13.891	-77.513	-36.203	10.549
800	33.370	73.746	54.314	15.546	-77.208	-33.460	9.141
823	33.609	74.693	54.868	16.316	-77.065	-32.202	8.551
823	48.011	86.496	54.868	26.030	-67.351	-32.202	8.551
850	47.337	88.036	55.892	27.317	-66.806	-31.057	7.985
900	46.092	90.705	57.757	29.653	-65.860	-28.980	7.037
903.9	45.995	90.904	57.900	29.833	-65.791	-28.820	6.968
903.9	45.995	90.904	57.900	29.833	-75.291	-28.820	6.968
950	44.845	93.165	59.558	31.927	-74.500	-26.465	6.088
1000	43.599	95.433	61.295	34.138	-73.704	-23.972	5.239
1050	42.352	97.529	62.970	36.287	-72.975	-21.491	4.473

Phase changes: 823 K, melting point of Sb_2S_3 ; $\Delta\text{H}^\circ = 9.714$ kcal/mol.
 903.9 K, melting point of Sb; $\Delta\text{H}^\circ = 4.750$ kcal/mol.

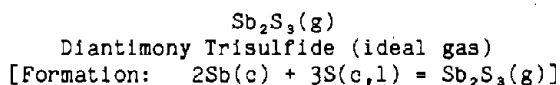
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-823 K: $\text{Cp}^\circ = 25.971 + 9.160 \times 10^{-3}T - 0.046 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 25.971 \times 10^{-3}T + 4.580 \times 10^{-6}T^2 + 0.046 \times 10^{-2}T^3 - 8.166$
 823-1050 K: $\text{Cp}^\circ = 69.133 - 25.366 \times 10^{-3}T - 1.662 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 69.133 \times 10^{-3}T - 12.683 \times 10^{-6}T^2 + 1.662 \times 10^{-2}T^3 - 22.478$

Reaction equations (kcal/mol):

298.15-823 K: $\Delta\text{Hr}^\circ = -80.906 + 3.280 \times 10^{-3}T + 1.756 \times 10^{-6}T^2 - 54.650T^{-1}$
 $\Delta\text{Gr}^\circ = -80.906 - 3.280 \times 10^{-3}T \ln T - 1.756 \times 10^{-6}T^2 - 27.325T^{-1} + 82.690 \times 10^{-3}T$
 823-903.9 K: $\Delta\text{Hr}^\circ = -95.218 + 46.443 \times 10^{-3}T - 15.507 \times 10^{-6}T^2 + 106.950T^{-1}$
 $\Delta\text{Gr}^\circ = -95.218 - 46.443 \times 10^{-3}T \ln T + 15.507 \times 10^{-6}T^2 + 53.475T^{-1} + 375.498 \times 10^{-3}T$
 903.9-1050 K: $\Delta\text{Hr}^\circ = -102.225 + 41.619 \times 10^{-3}T - 13.163 \times 10^{-6}T^2 + 63.750T^{-1}$
 $\Delta\text{Gr}^\circ = -102.225 - 41.619 \times 10^{-3}T \ln T + 13.163 \times 10^{-6}T^2 + 31.875T^{-1} + 352.560 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K and high-temperature data from Johnson (56). Low-temperature heat capacities and entropy at 298 from King (68).



T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15*	23.789	97.921	97.921	0	28.600	12.745	-9.342
300	23.811	98.068	97.921	.044	28.592	12.649	-9.215
368.3	24.362	103.021	98.422	1.694	28.257	9.053	-5.372
368.3	24.362	103.021	98.422	1.694	27.969	9.053	-5.372
388.36	24.524	104.317	98.694	2.184	27.855	8.027	-4.517
388.36	24.524	104.317	98.694	2.184	26.616	8.027	-4.517
400	24.618	105.043	98.868	2.470	26.494	7.472	-4.082
432.02	24.750	106.944	99.397	3.260	26.097	5.962	-3.016
500	25.030	110.585	100.675	4.955	24.914	2.897	-1.266
600	25.265	115.171	102.719	7.471	23.579	-1.384	.504
700	25.412	119.077	104.784	10.005	22.395	-5.443	1.699
717.824	25.429	119.716	105.147	10.458	22.197	-6.148	1.872

*Data except enthalpy of formation at 298 K estimated.

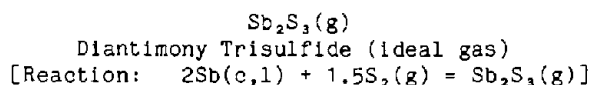
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-3000 K: $C_p^\circ = 25.725 + 0.050 \times 10^{-3}T - 1.734 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 25.725 \times 10^{-3}T + 0.025 \times 10^{-6}T^2 + 1.734 \times 10^{-2}T^{-1} - 8.254$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 31.863 - 8.973 \times 10^{-3}T + 2.832 \times 10^{-6}T^2 - 250.200T^{-1}$
 $\Delta G_f^\circ = 31.863 + 8.973 \times 10^{-3}T \ln T - 2.832 \times 10^{-6}T^2 - 125.100T^{-1} - 112.994 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = 28.517 - 2.184 \times 10^{-3}T - 2.406 \times 10^{-6}T^2 + 216.600T^{-1}$
 $\Delta G_f^\circ = 28.517 + 2.184 \times 10^{-3}T \ln T + 2.406 \times 10^{-6}T^2 + 108.300T^{-1} - 67.445 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -19.958 + 132.036 \times 10^{-3}T - 132.252 \times 10^{-6}T^2 + 5923.200T^{-1}$
 $\Delta G_f^\circ = -19.958 - 132.036 \times 10^{-3}T \ln T + 132.252 \times 10^{-6}T^2 + 2961.600T^{-1} + 788.240 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -48.394 + 120.318 \times 10^{-3}T - 72.816 \times 10^{-6}T^2 + 15602.700T^{-1}$
 $\Delta G_f^\circ = -48.394 - 120.318 \times 10^{-3}T \ln T + 72.816 \times 10^{-6}T^2 + 7801.350T^{-1} + 782.697 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15*	23.789	97.921	97.921	0	-17.465	-15.796	11.579
300	23.811	98.068	97.921	.044	-17.464	-15.783	11.498
400	24.618	105.043	98.868	2.470	-17.459	-15.225	8.319
500	25.030	110.585	100.675	4.955	-17.468	-14.663	6.409
600	25.265	115.171	102.719	7.471	-17.504	-14.107	5.138
700	25.412	119.077	104.784	10.005	-17.580	-13.529	4.224
800	25.508	122.477	106.788	12.551	-17.713	-12.950	3.538
900	25.575	125.486	108.702	15.106	-17.917	-12.340	2.997
903.9	25.577	125.597	108.774	15.206	-17.927	-12.316	2.978
903.9	25.577	125.597	108.774	15.206	-27.427	-12.316	2.978
1000	25.623	128.183	110.517	17.666	-27.686	-10.704	2.339
1100	25.659	130.627	112.236	20.230	-27.965	-8.981	1.784
1200	25.687	132.861	113.863	22.797	-28.251	-7.249	1.320
1300	25.708	134.918	115.405	25.367	-28.544	-5.488	.923
1400	25.726	136.824	116.868	27.939	-28.848	-3.691	.576
1500	25.739	138.599	118.258	30.512	-29.161	-1.876	.273
1600	25.751	140.261	119.582	33.087	-29.482	-.060	.008
1700	25.760	141.822	120.844	35.662	-29.816	1.773	-.228
1800	25.768	143.295	122.051	38.239	-30.155	3.647	-.443
1860	25.772	144.140	122.750	39.785	-30.363	4.792	-.563

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 903.9 K, melting point of Sb; $\Delta H^\circ = 4.750$ kcal/mol.

1860 K, boiling point of Sb to equilibrium mixture of $\text{Sb}(\text{g})$, $\text{Sb}_2(\text{g})$, and $\text{Sb}_3(\text{g})$.

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

298.15-3000 K: $C_p^\circ = 25.725 + 0.050 \times 10^{-3}T - 1.734 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 25.725 \times 10^{-3}T + 0.025 \times 10^{-6}T^2 + 1.734 \times 10^{-2}T^{-1} - 8.254$

Reaction equations (kcal/mol):

298.15-903.9 K: $\Delta H_r^\circ = -18.504 + 3.034 \times 10^{-3}T - 2.799 \times 10^{-6}T^2 + 114.150T^{-1}$
 $\Delta G_r^\circ = -18.504 - 3.034 \times 10^{-3}T \ln T + 2.799 \times 10^{-6}T^2 + 57.075T^{-1} + 24.895 \times 10^{-3}T$
 903.9-1860 K: $\Delta H_r^\circ = -25.511 - 1.790 \times 10^{-3}T + 0.455 \times 10^{-6}T^2 + 70.950T^{-1}$
 $\Delta G_r^\circ = -25.511 + 1.790 \times 10^{-3}T \ln T + 0.455 \times 10^{-6}T^2 + 35.475T^{-1} + 1.956 \times 10^{-3}T$

Source: Data based on Prusaczyk (101) who estimated molecular constants.

Sb₂S₄(g)
Diantimony Tetrasulfide (ideal gas)
[Formation: 2Sb(c) + 4S(c,l) = Sb₂S₄(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H _{2,98} °)/T	H°- H _{2,98} °	ΔHf°	ΔGf°	
298.15*	29.328	103.282	103.282	0	22.400	7.231	-5.300
300	29.354	103.464	103.284	.054	22.392	7.139	-5.201
368.3	30.025	109.569	103.899	2.088	22.058	3.699	-2.195
368.3	30.025	109.569	103.899	2.088	21.674	3.699	-2.195
388.36	30.223	111.167	104.234	2.693	21.555	2.726	-1.534
388.36	30.223	111.167	104.234	2.693	19.903	2.726	-1.534
400	30.337	112.061	104.448	3.045	19.759	2.213	-1.209
432.02	30.496	114.403	105.101	4.019	19.283	.824	-.417
500	30.835	118.889	106.677	6.106	17.818	-1.952	.853
600	31.117	124.538	109.196	9.205	16.209	-5.757	2.097
700	31.292	129.349	111.740	12.326	14.812	-9.299	2.903
717.824	31.313	130.136	112.187	12.884	14.582	-9.908	3.017

*Data except enthalpy of formation at 298 K estimated.

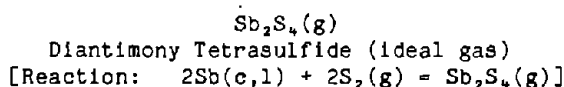
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-3000 K: Cp° = 31.676 + 0.056x10⁻³T - 2.102x10⁻⁵T⁻²
H°- H_{2,98}° = 31.676x10⁻³T + 0.028x10⁻⁵T² + 2.102x10⁻²T⁻¹ - 10.152

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 26.571 - 11.196x10⁻³T + 4.552x10⁻⁶T² - 369.000T⁻¹
ΔGf° = 26.571 + 11.196x10⁻³TlnT - 4.552x10⁻⁶T² - 184.500T⁻¹ - 125.225x10⁻³T
368.3-388.36 K: ΔHf° = 22.111 - 2.144x10⁻³T - 2.432x10⁻⁶T² + 253.400T⁻¹
ΔGf° = 22.111 + 2.144x10⁻³TlnT + 2.432x10⁻⁶T² + 126.700T⁻¹ - 64.494x10⁻³T
388.36-432.02 K: ΔHf° = -42.523 + 176.816x10⁻³T - 175.560x10⁻⁶T² + 7862.200T⁻¹
ΔGf° = -42.523 - 176.816x10⁻³TlnT + 175.560x10⁻⁶T² + 3931.100T⁻¹ + 1076.420x10⁻³T
432.02-717.824 K: ΔHf° = -80.437 + 161.192x10⁻³T - 96.312x10⁻⁶T² + 20768.200T⁻¹
ΔGf° = -80.437 + 161.192x10⁻³TlnT + 96.312x10⁻⁶T² + 10384.100T⁻¹ + 1069.030x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHr°	ΔGr°	
298.15*	29.328	103.282	103.282	0	-39.020	-30.824	22.594
300	29.354	103.464	103.284	.054	-39.016	-30.770	22.416
400	30.337	112.061	104.448	3.045	-38.845	-28.049	15.325
500	30.835	118.889	106.677	6.106	-38.692	-25.365	11.087
600	31.117	124.538	109.196	9.205	-38.569	-22.721	8.276
700	31.292	129.349	111.740	12.326	-38.488	-20.080	6.269
800	31.408	133.536	114.210	15.461	-38.467	-17.461	4.770
900	31.488	137.240	116.567	18.606	-38.522	-14.830	3.601
903.9	31.490	137.376	116.656	18.729	-38.526	-14.728	3.561
903.9	31.490	137.376	116.656	18.729	-48.026	-14.728	3.561
1000	31.545	140.561	118.803	21.758	-48.142	-11.189	2.445
1100	31.588	143.569	120.919	24.915	-48.275	-7.475	1.485
1200	31.621	146.319	122.923	28.075	-48.419	-3.766	.686
1300	31.646	148.851	124.821	31.239	-48.573	-.040	.007
1400	31.667	151.197	126.622	34.405	-48.741	3.713	-.580
1500	31.683	153.383	128.335	37.572	-48.922	7.470	-1.088
1600	31.697	155.428	129.965	40.741	-49.115	11.224	-1.533
1700	31.708	157.350	131.520	43.911	-49.323	14.985	-1.926
1800	31.717	159.163	133.006	47.083	-49.539	18.780	-2.280
1860	31.722	160.203	133.866	48.986	-49.676	21.074	-2.476

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 903.9 K, melting point of Sb; $\Delta\text{H}^\circ = 4.750$ kcal/mol.

1860 K, boiling point of Sb to equilibrium mixture of $\text{Sb}(\text{g})$, $\text{Sb}_2(\text{g})$, and $\text{Sb}_4(\text{g})$.

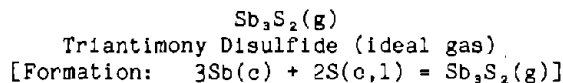
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $\text{Cp}^\circ = 31.676 + 0.056 \times 10^{-3}T - 2.102 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 31.676 \times 10^{-3}T + 0.028 \times 10^{-6}T^2 + 2.102 \times 10^{-2}T^{-1} - 10.152$

Reaction equations (kcal/mol):

298.15-903.9 K: $\Delta\text{Hr}^\circ = -40.584 + 4.814 \times 10^{-3}T - 2.956 \times 10^{-6}T^2 + 116.800T^{-1}$
 $\Delta\text{Gr}^\circ = -40.584 - 4.814 \times 10^{-3}T \ln T + 2.956 \times 10^{-6}T^2 + 58.400T^{-1} + 58.627 \times 10^{-3}T$
 903.9-1860 K: $\Delta\text{Hr}^\circ = -47.591 - 0.010 \times 10^{-3}T - 0.612 \times 10^{-6}T^2 + 73.600T^{-1}$
 $\Delta\text{Gr}^\circ = -47.591 + 0.010 \times 10^{-3}T \ln T + 0.612 \times 10^{-6}T^2 + 36.800T^{-1} + 35.688 \times 10^{-3}T$

Source: Data based on Prusaczyk (101) who estimated molecular constants.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	23.461	97.101	97.101	0	37.600	22.949	-16.822
300	23.486	97.246	97.103	.043	37.590	22.861	-16.654
368.3	24.131	102.143	97.594	1.675	37.205	19.549	-11.600
368.3	24.131	102.143	97.594	1.675	37.013	19.549	-11.600
388.36	24.320	103.428	97.863	2.161	36.890	18.602	-10.468
388.36	24.320	103.428	97.863	2.161	36.064	18.602	-10.468
400	24.430	104.148	98.035	2.445	35.956	18.080	-9.878
432.02	24.583	106.035	98.559	3.230	35.617	16.661	-8.428
500	24.908	109.657	99.829	4.914	34.670	13.759	-6.014
600	25.180	114.224	101.857	7.420	33.542	9.674	-3.524
700	25.349	118.119	103.909	9.947	32.492	5.789	-1.807
717.824	25.369	118.756	104.270	10.399	32.310	5.113	-1.557

*Data except enthalpy of formation at 298 K estimated.

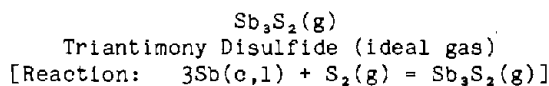
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-3000 K: $\text{Cp}^\circ = 25.718 + 0.054 \times 10^{-3}T - 2.021 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 25.718 \times 10^{-3}T + 0.027 \times 10^{-6}T^2 + 2.021 \times 10^{-2}T^{-1} - 8.348$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta \text{Hf}^\circ = 39.511 - 5.894 \times 10^{-3}T - 0.055 \times 10^{-6}T^2 - 44.300T^{-1}$
 $\Delta \text{Gf}^\circ = 39.511 + 5.894 \times 10^{-3}T \ln T + 0.055 \times 10^{-6}T^2 - 22.150T^{-1} - 88.897 \times 10^{-3}T$
 368.3-388.36 K: $\Delta \text{Hf}^\circ = 37.281 - 1.368 \times 10^{-3}T - 3.547 \times 10^{-6}T^2 + 266.900T^{-1}$
 $\Delta \text{Gf}^\circ = 37.281 + 1.368 \times 10^{-3}T \ln T + 3.547 \times 10^{-6}T^2 + 133.450T^{-1} - 58.531 \times 10^{-3}T$
 388.36-432.02 K: $\Delta \text{Hf}^\circ = 4.964 + 88.112 \times 10^{-3}T - 90.111 \times 10^{-6}T^2 + 4071.300T^{-1}$
 $\Delta \text{Gf}^\circ = 4.964 - 88.112 \times 10^{-3}T \ln T + 90.111 \times 10^{-6}T^2 + 2035.650T^{-1} + 511.926 \times 10^{-3}T$
 432.02-717.824 K: $\Delta \text{Hf}^\circ = -13.993 + 80.300 \times 10^{-3}T - 50.487 \times 10^{-6}T^2 + 10524.300T^{-1}$
 $\Delta \text{Gf}^\circ = -13.993 - 80.300 \times 10^{-3}T \ln T + 50.487 \times 10^{-6}T^2 + 5262.150T^{-1} + 508.231 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15*	23.461	97.101	97.101	0	6.890	3.922	-2.875
300	23.486	97.246	97.103	.043	6.886	3.907	-2.846
400	24.430	104.148	98.035	2.445	6.654	2.949	-1.611
500	24.908	109.657	99.829	4.914	6.415	2.052	-.897
600	25.180	114.224	101.857	7.420	6.153	1.192	-.434
700	25.349	118.119	103.909	9.947	5.842	.399	-.125
800	25.460	121.512	105.902	12.488	5.454	-.366	.100
900	25.537	124.515	107.806	15.038	4.964	-1.060	.257
903.9	25.539	124.625	107.878	15.138	4.942	-1.085	.262
903.9	25.539	124.625	107.878	15.138	-9.308	-1.085	.262
1000	25.593	127.209	109.614	17.595	-9.863	-.195	.043
1100	25.634	129.650	111.326	20.156	-10.447	.817	-.162
1200	25.666	131.882	112.948	22.721	-11.034	1.858	-.338
1300	25.690	133.937	114.484	25.289	-11.625	2.955	-.497
1400	25.710	135.842	115.943	27.859	-12.222	4.116	-.643
1500	25.726	137.616	117.329	30.431	-12.824	5.315	-.774
1600	25.739	139.277	118.649	33.004	-13.432	6.525	-.891
1700	25.749	140.838	119.910	35.578	-14.047	7.766	-.998
1800	25.758	142.310	121.113	38.154	-14.665	9.075	-1.102
1860	25.763	143.155	121.811	39.699	-15.039	9.895	-1.163

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 903.9 K, melting point of Sb; $\Delta H^\circ = 4.750$ kcal/mol.

1860 K, boiling point of Sb to equilibrium mixture of $\text{Sb}(\text{g})$, $\text{Sb}_2(\text{g})$, and $\text{Sb}_3(\text{g})$.

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

298.15-3000 K: $C_p^\circ = 25.718 + 0.054 \times 10^{-3}T - 2.021 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 25.718 \times 10^{-3}T + 0.027 \times 10^{-6}T^2 + 2.021 \times 10^{-2}T^3 - 8.348$

Reaction equations (kcal/mol):

298.15-903.9 K: $\Delta H_r^\circ = 5.933 + 2.111 \times 10^{-3}T - 3.809 \times 10^{-6}T^2 + 198.600T^{-1}$
 $\Delta G_r^\circ = 5.933 - 2.111 \times 10^{-3}T \ln T + 3.809 \times 10^{-6}T^2 + 99.300T^{-1} + 3.029 \times 10^{-3}T$
 903.9-1860 K: $\Delta H_r^\circ = -4.577 - 5.125 \times 10^{-3}T - 0.293 \times 10^{-6}T^2 + 133.800T^{-1}$
 $\Delta G_r^\circ = -4.577 + 5.125 \times 10^{-3}T \ln T + 0.293 \times 10^{-6}T^2 + 66.900T^{-1} - 31.378 \times 10^{-3}T$

Source: Data based on Prusaczyk (101) who estimated molecular constants.

Sb₄S₃(g)
Tetraantimony Trisulfide (ideal gas)
[Formation: 4Sb(c) + 3S(c,l) = Sb₄S₃(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H _{2,98} °)/T	H° - H _{2,98} °	ΔHf°	ΔGf°	
298.15*	35.273	115.465	115.465	0	37.600	23.002	-16.861
300	35.301	115.683	115.466	.065	37.591	22.916	-16.694
368.3	36.001	123.012	116.206	2.507	37.215	19.613	-11.638
368.3	36.001	123.012	116.206	2.507	36.927	19.613	-11.638
388.36	36.207	124.927	116.608	3.231	36.800	18.676	-10.510
388.36	36.207	124.927	116.608	3.231	35.561	18.676	-10.510
400	36.326	125.998	116.866	3.653	35.431	18.171	-9.928
432.02	36.486	128.802	117.648	4.819	35.011	16.803	-8.500
500	36.826	134.164	119.536	7.314	33.773	14.046	-6.140
600	37.104	140.905	122.553	11.011	32.339	10.224	-3.724
700	37.275	146.638	125.594	14.731	31.023	6.656	-2.078
717.824	37.295	147.575	126.128	15.395	30.796	6.040	-1.839

*Data except enthalpy of formation at 298 K estimated.

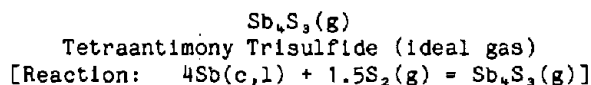
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-3000 K: Cp° = 37.689 + 0.032x10⁻³T - 2.156x10⁻⁵T⁻²
H° - H_{2,98}° = 37.689x10⁻³T + 0.016x10⁻⁶T² + 2.156x10⁻²T⁻¹ - 11.962

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 40.252 - 7.185x10⁻³T + 0.479x10⁻⁶T² - 164.800T⁻¹
ΔGf° = 40.252 + 7.185x10⁻³TlnT - 0.479x10⁻⁶T² - 82.400T⁻¹ - 97.726x10⁻³T
368.3-388.36 K: ΔHf° = 36.907 - 0.396x10⁻³T - 4.759x10⁻⁶T² + 302.000T⁻¹
ΔGf° = 36.907 + 0.396x10⁻³TlnT + 4.759x10⁻⁶T² + 151.000T⁻¹ - 52.177x10⁻³T
388.36-432.02 K: ΔHf° = -11.568 + 133.824x10⁻³T - 134.605x10⁻⁶T² + 6008.600T⁻¹
ΔGf° = -11.568 - 133.824x10⁻³TlnT + 134.605x10⁻⁶T² + 3004.300T⁻¹ + 803.508x10⁻³T
432.02-717.824 K: ΔHf° = -40.004 + 122.106x10⁻³T - 75.169x10⁻⁶T² + 15688.100T⁻¹
ΔGf° = -40.004 - 122.106x10⁻³TlnT + 75.169x10⁻⁶T² + 7844.050T⁻¹ + 797.966x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHr°	ΔGr°	
298.15*	35.273	115.465	115.465	0	-8.465	-5.539	4.060
300	35.301	115.683	115.466	.065	-8.465	-5.516	4.018
400	36.326	125.998	116.866	3.653	-8.522	-4.526	2.473
500	36.826	134.164	119.536	7.314	-8.610	-3.513	1.536
600	37.104	140.905	122.553	11.011	-8.744	-2.499	.910
700	37.275	146.638	125.594	14.731	-8.952	-1.429	.446
800	37.386	151.623	128.543	18.464	-9.270	-.351	.096
900	37.463	156.032	131.358	22.207	-9.727	.795	-.193
903.9	37.465	156.194	131.464	22.353	-9.748	.842	-.204
903.9	37.465	156.194	131.464	22.353	-28.748	.842	-.204
1000	37.519	159.982	134.026	25.956	-29.304	4.000	-.874
1100	37.560	163.560	136.551	29.710	-29.893	7.381	-1.466
1200	37.591	166.829	138.939	33.468	-30.488	10.785	-1.964
1300	37.615	169.839	141.202	37.228	-31.091	14.245	-2.395
1400	37.635	172.628	143.349	40.991	-31.703	17.780	-2.775
1500	37.650	175.225	145.388	44.755	-32.326	21.350	-3.111
1600	37.663	177.655	147.329	48.521	-32.956	24.924	-3.404
1700	37.674	179.939	149.181	52.288	-33.598	28.528	-3.668
1800	37.683	182.092	150.950	56.056	-34.246	32.213	-3.911
1860	37.687	183.328	151.975	58.316	-34.640	34.463	-4.049

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 903.9 K, melting point of Sb; $\Delta\text{H}^\circ = 4.750$ kcal/mol.

1860 K, boiling point of Sb to equilibrium mixture of $\text{Sb}(\text{g})$, $\text{Sb}_2(\text{g})$, and $\text{Sb}_4(\text{g})$.

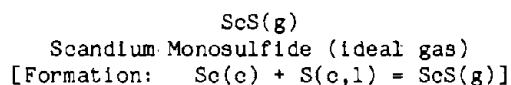
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-3000 K: $\text{Cp}^\circ = 37.689 + 0.032 \times 10^{-3}T - 2.156 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 37.689 \times 10^{-3}T + 0.016 \times 10^{-6}T^2 + 2.156 \times 10^{-2}T^{-1} - 11.962$

Reaction equations (kcal/mol):

298.15-903.9 K: $\Delta\text{Hr}^\circ = -10.114 + 4.823 \times 10^{-3}T - 5.152 \times 10^{-6}T^2 + 199.550T^{-1}$
 $\Delta\text{Gr}^\circ = -10.114 - 4.823 \times 10^{-3}T \ln T + 5.152 \times 10^{-6}T^2 + 99.775T^{-1} + 40.163 \times 10^{-3}T$
 903.9-1860 K: $\Delta\text{Hr}^\circ = -24.128 - 4.825 \times 10^{-3}T - 0.464 \times 10^{-6}T^2 + 113.150T^{-1}$
 $\Delta\text{Gr}^\circ = -24.128 + 4.825 \times 10^{-3}T \ln T + 0.464 \times 10^{-6}T^2 + 56.575T^{-1} - 5.714 \times 10^{-3}T$

Source: Data based on Prusaczyk (101) who estimated molecular constants.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	8.010	56.540	56.540	0	43.300	31.195	-22.867
300	8.020	56.590	56.540	.015	43.294	31.121	-22.672
368.3	8.273	58.262	56.704	.574	43.046	28.376	-16.838
368.3	8.273	58.262	56.704	.574	42.950	28.376	-16.838
388.36	8.347	58.703	56.796	.741	42.873	27.585	-15.523
388.36	8.347	58.703	56.796	.741	42.460	27.585	-15.523
400	8.390	58.950	56.855	.838	42.396	27.140	-14.828
432.02	8.444	59.598	57.035	1.108	42.201	25.925	-13.115
500	8.560	60.850	57.476	1.687	41.673	23.407	-10.231
600	8.660	62.420	58.173	2.548	41.028	19.813	-7.217
700	8.720	63.760	58.879	3.417	40.431	16.327	-5.098
717.824	8.727	63.979	59.002	3.572	40.329	15.715	-4.785

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.

388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.

432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.

717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 8.828 + 0.060x10⁻³T - 0.740x10⁻⁵T²
H° - H°₂₉₈ = 8.828x10⁻³T + 0.030x10⁻⁶T² + 0.740x10⁻⁵T³ - 2.883

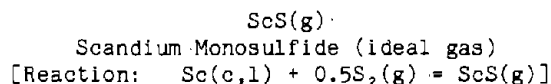
Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 44.674 - 4.230x10⁻³T + 0.408x10⁻⁶T² - 44.500T⁻¹
ΔGf° = 44.674 + 4.230x10⁻³T lnT - 0.408x10⁻⁶T² - 22.250T⁻¹ - 68.937x10⁻³T

368.3-388.36 K: ΔHf° = 43.559 - 1.967x10⁻³T - 1.338x10⁻⁶T² + 111.100T⁻¹
ΔGf° = 43.559 + 1.967x10⁻³T lnT + 1.338x10⁻⁶T² + 55.550T⁻¹ - 53.754x10⁻³T

388.36-432.02 K: ΔHf° = 27.401 + 42.773x10⁻³T - 44.620x10⁻⁶T² + 2013.300T⁻¹
ΔGf° = 27.401 - 42.773x10⁻³T lnT + 44.620x10⁻⁶T² + 1006.650T⁻¹ + 231.474x10⁻³T

432.02-717.824 K: ΔHf° = 17.922 + 38.867x10⁻³T - 24.808x10⁻⁶T² + 5239.800T⁻¹
ΔGf° = 17.922 - 38.867x10⁻³T lnT + 24.808x10⁻⁶T² + 2619.900T⁻¹ + 229.627x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15*	8.010	56.540	56.540	0	27.945	21.682	-15.893
300	8.020	56.590	56.540	.015	27.942	21.644	-15.768
400	8.390	58.950	56.855	.838	27.745	19.574	-10.695
500	8.560	60.850	57.476	1.687	27.545	17.553	-7.672
600	8.660	62.420	58.173	2.548	27.333	15.572	-5.672
700	8.720	63.760	58.879	3.417	27.106	13.632	-4.256
800	8.760	64.920	59.556	4.291	26.859	11.734	-3.206
900	8.790	65.960	60.217	5.169	26.589	9.841	-2.390
1000	8.810	66.890	60.841	6.049	26.293	7.992	-1.747
1100	8.830	67.730	61.429	6.931	25.967	6.184	-1.229
1200	8.850	68.500	61.987	7.815	25.610	4.427	-.806
1300	8.860	69.200	62.507	8.701	25.220	2.666	-.448
1400	8.870	69.860	63.011	9.588	24.791	.936	-.146
1500	8.880	70.470	63.486	10.476	24.323	-.743	.108
1600	8.890	71.050	63.947	11.365	23.812	-2.412	.329
1608	8.891	71.094	63.982	11.436	23.770	-2.536	.345
1608	8.891	71.094	63.982	11.436	22.812	-2.536	.345
1700	8.900	71.590	64.381	12.255	22.227	-3.980	.512
1800	8.910	72.100	64.797	13.146	21.588	-5.511	.669
1812	8.911	72.159	64.845	13.253	21.512	-5.691	.686
1812	8.911	72.159	64.845	13.253	18.143	-5.691	.686
1900	8.920	72.580	65.192	14.037	17.578	-6.834	.786
2000	8.930	73.040	65.575	14.930	16.935	-8.111	.886

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1608 K, α - β transition point of Sc; ΔH° = 0.958 kcal/mol.
1812 K, melting point of Sc; ΔH° = 3.369 kcal/mol.

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

298.15-2000 K: $C_p^\circ = 8.828 + 0.060 \times 10^{-3}T - 0.740 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 8.828 \times 10^{-3}T + 0.030 \times 10^{-6}T^2 + 0.740 \times 10^{-2}T^{-1} - 2.883$

Reaction equations (kcal/mol):

298.15-1608 K: $\Delta H_r^\circ = 27.885 - 0.227 \times 10^{-3}T - 1.469 \times 10^{-6}T^2 + 76.950T^{-1}$
 $\Delta G_r^\circ = 27.885 + 0.227 \times 10^{-3}T \ln T + 1.469 \times 10^{-6}T^2 + 38.475T^{-1} - 22.974 \times 10^{-3}T$
1608-1812 K: $\Delta H_r^\circ = 32.631 - 5.913 \times 10^{-3}T - 0.130 \times 10^{-6}T^2 + 39.850T^{-1}$
 $\Delta G_r^\circ = 32.631 + 5.913 \times 10^{-3}T \ln T + 0.130 \times 10^{-6}T^2 + 19.925T^{-1} - 65.743 \times 10^{-3}T$
1812-2000 K: $\Delta H_r^\circ = 29.262 - 5.913 \times 10^{-3}T - 0.130 \times 10^{-6}T^2 + 39.850T^{-1}$
 $\Delta G_r^\circ = 29.262 + 5.913 \times 10^{-3}T \ln T + 0.130 \times 10^{-6}T^2 + 19.925T^{-1} - 63.884 \times 10^{-3}T$

Source: Data from Mills (80) who estimated all except enthalpy of formation at 298 K.

SiS(c)
Silicon Monosulfide
[Formation: Si(c) + S(c,l) = SiS(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15*	10.750	15.060	15.060	0	-40.400	-41.264	30.247
300	10.760	15.120	15.060	.020	-40.399	-41.268	30.063
368.3	11.006	17.357	15.295	.759	-40.385	-41.476	24.612
368.3	11.006	17.357	15.295	.759	-40.481	-41.476	24.612
388.36	11.078	17.942	15.417	.981	-40.483	-41.529	23.370
388.36	11.078	17.942	15.417	.981	-40.896	-41.529	23.370
400	11.120	18.270	15.495	1.110	-40.916	-41.548	22.701
432.02	11.235	19.131	15.733	1.468	-40.992	-41.597	21.043
500	11.480	20.790	16.310	2.240	-41.269	-41.666	18.212
600	11.840	22.910	17.227	3.410	-41.528	-41.713	15.194
700	12.200	24.770	18.184	4.610	-41.719	-41.736	13.030
717.824	12.264	25.077	18.352	4.828	-41.745	-41.735	12.707

*Data except enthalpy of formation at 298 K estimated.

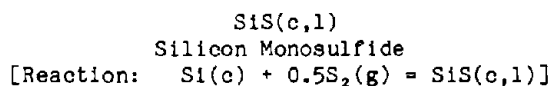
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1363 K: Cp° = 9.665 + 3.614x10⁻³T + 0.006x10⁻⁵T⁻²
H°- H₂₉₈° = 9.665x10⁻³T + 1.807x10⁻⁶T² - 0.006x10⁻²T⁻¹ - 3.040

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -38.579 - 4.188x10⁻³T + 3.173x10⁻⁶T² - 254.700T⁻¹
ΔGf° = -38.579 + 4.188x10⁻³TlnT - 3.173x10⁻⁶T² - 127.350T⁻¹ - 30.489x10⁻³T
368.3-388.36 K: ΔHf° = -39.694 - 1.925x10⁻³T + 1.427x10⁻⁶T² - 99.100T⁻¹
ΔGf° = -39.694 + 1.925x10⁻³TlnT - 1.427x10⁻⁶T² - 49.550T⁻¹ - 15.306x10⁻³T
388.36-432.02 K: ΔHf° = -55.853 + 42.815x10⁻³T - 41.855x10⁻⁶T² + 1803.100T⁻¹
ΔGf° = -55.853 - 42.815x10⁻³TlnT + 41.855x10⁻⁶T² + 901.550T⁻¹ + 269.922x10⁻³T
432.02-717.824 K: ΔHf° = -65.331 + 38.909x10⁻³T - 22.043x10⁻⁶T² + 5029.600T⁻¹
ΔGf° = -65.331 - 38.909x10⁻³TlnT + 22.043x10⁻⁶T² + 2514.800T⁻¹ + 268.075x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	10.750	15.060	15.060	0	-55.755	-50.778	37.221
300	10.760	15.120	15.060	.020	-55.751	-50.745	36.967
400	11.120	18.270	15.495	1.110	-55.567	-49.114	26.834
500	11.480	20.790	16.310	2.240	-55.396	-47.519	20.770
600	11.840	22.910	17.227	3.410	-55.223	-45.954	16.738
700	12.200	24.770	18.184	4.610	-55.044	-44.431	13.872
800	12.560	26.420	19.108	5.850	-54.845	-42.922	11.726
900	12.920	27.920	20.009	7.120	-54.635	-41.449	10.065
1000	13.280	29.300	20.870	8.430	-54.396	-39.988	8.739
1100	13.630	30.580	21.689	9.780	-54.131	-38.560	7.661
1200	13.990	31.780	22.480	11.160	-53.846	-37.157	6.767
1300	14.350	32.920	23.243	12.580	-53.530	-35.784	6.016
1363	14.580	33.600	23.704	13.490	-53.322	-34.922	5.599
1363	16.000	39.040	23.704	20.900	-45.912	-34.922	5.599
1400	16.000	39.460	24.110	21.490	-45.736	-34.618	5.404
1500	16.000	40.570	25.177	23.090	-45.261	-33.861	4.934
1600	16.000	41.600	26.169	24.690	-44.794	-33.114	4.523

*Data except enthalpy of formation at 298 K estimated.

Phase change: 1363 K, melting point of SiS; $\Delta H^\circ = 7.41$ kcal/mol.

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

298.15-1363 K: $C_p^\circ = 9.665 + 3.614 \times 10^{-3}T + 0.006 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 9.665 \times 10^{-3}T + 1.807 \times 10^{-6}T^2 - 0.006 \times 10^{-2}T^{-1} - 3.040$
 1363-1600 K: $C_p^\circ = 16.000$
 $H^\circ - H_{298}^\circ = 16.000 \times 10^{-3}T - 0.908$

Reaction equations (kcal/mol):

298.15-1363 K: $\Delta H_r^\circ = -55.368 - 0.185 \times 10^{-3}T + 1.296 \times 10^{-6}T^2 - 133.250T^{-1}$
 $\Delta G_r^\circ = -55.368 + 0.185 \times 10^{-3}T \ln T - 1.296 \times 10^{-6}T^2 - 66.625T^{-1} + 15.474 \times 10^{-3}T$
 1363-1600 K: $\Delta H_r^\circ = -53.236 + 6.150 \times 10^{-3}T - 0.511 \times 10^{-6}T^2 - 132.650T^{-1}$
 $\Delta G_r^\circ = -53.236 - 6.150 \times 10^{-3}T \ln T + 0.511 \times 10^{-6}T^2 - 66.325T^{-1} + 57.169 \times 10^{-3}T$

Source: Data from Gurvich (49) who estimated all except enthalpy of formation at 298 K.

SiS(g)
Silicon Monosulfide (ideal gas)
[Formation: Si(c) + S(c,l) = SiS(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	7.728	53.462	53.462	0	25.320	13.006	-9.534
300	7.736	53.510	53.463	.014	25.315	12.930	-9.419
368.3	7.995	55.126	53.625	.553	25.128	10.127	-6.009
368.3	7.995	55.126	53.625	.553	25.032	10.127	-6.009
388.36	8.071	55.552	53.714	.714	24.970	9.317	-5.243
388.36	8.071	55.552	53.714	.714	24.557	9.317	-5.243
400	8.115	55.791	53.771	.808	24.502	8.861	-4.841
432.02	8.195	56.419	53.944	1.069	24.329	7.615	-3.852
500	8.364	57.631	54.365	1.633	23.844	5.027	-2.197
600	8.528	59.171	55.041	2.478	23.260	1.319	-.480
700	8.639	60.495	55.728	3.337	22.728	-2.296	.717
717.824	8.653	60.712	55.849	3.491	22.638	-2.932	.893

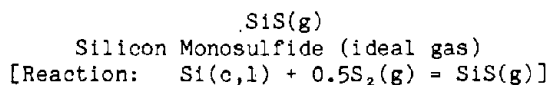
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 8.589 + 0.274x10⁻³T - 0.838x10⁻⁵T⁻²
H° - H°₂₉₈ = 8.589x10⁻³T + 0.137x10⁻⁶T² + 0.838x10⁻²T⁻¹ - 2.854

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 27.327 - 5.264x10⁻³T + 1.503x10⁻⁶T² - 170.300T⁻¹
ΔGf° = 27.327 + 5.264x10⁻³T ln T - 1.503x10⁻⁶T² - 85.150T⁻¹ - 76.619x10⁻³T
368.3-388.36 K: ΔHf° = 26.212 - 3.001x10⁻³T - 0.243x10⁻⁶T² - 14.700T⁻¹
ΔGf° = 26.212 + 3.001x10⁻³T ln T + 0.243x10⁻⁶T² - 7.350T⁻¹ - 61.436x10⁻³T
388.36-432.02 K: ΔHf° = 10.054 + 41.739x10⁻³T - 43.525x10⁻⁶T² + 1887.500T⁻¹
ΔGf° = 10.054 - 41.739x10⁻³T ln T + 43.525x10⁻⁶T² + 943.750T⁻¹ + 223.793x10⁻³T
432.02-717.824 K: ΔHf° = 0.575 + 37.833x10⁻³T - 23.713x10⁻⁶T² + 5114.000T⁻¹
ΔGf° = 0.575 - 37.833x10⁻³T ln T + 23.713x10⁻⁶T² + 2557.000T⁻¹ + 221.945x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	7.728	53.462	53.462	0	9.965	3.492	-2.560
300	7.736	53.510	53.463	.014	9.963	3.452	-2.515
400	8.115	55.791	53.771	.808	9.851	1.296	-.708
500	8.364	57.631	54.365	1.633	9.716	-.826	.361
600	8.528	59.171	55.041	2.478	9.566	-2.922	1.064
700	8.639	60.495	55.728	3.337	9.403	-4.991	1.558
800	8.718	61.654	56.398	4.205	9.230	-7.034	1.922
900	8.777	62.684	57.040	5.080	9.045	-9.056	2.199
1000	8.821	63.611	57.651	5.960	8.854	-11.049	2.415
1100	8.856	64.454	58.232	6.844	8.654	-13.037	2.590
1200	8.884	65.225	58.782	7.731	8.445	-15.000	2.732
1300	8.908	65.938	59.307	8.620	8.230	-16.947	2.849
1400	8.928	66.598	59.804	9.512	8.007	-18.869	2.946
1500	8.945	67.215	60.278	10.406	7.776	-20.793	3.029
1600	8.960	67.793	60.730	11.301	7.537	-22.692	3.100
1687	8.972	68.267	61.106	12.081	7.323	-24.308	3.149
1687	8.972	68.267	61.106	12.081	-4.759	-24.308	3.149
1700	8.974	68.336	61.161	12.198	-4.782	-24.454	3.144
1800	8.986	68.850	61.574	13.096	-4.966	-25.604	3.109
1900	8.998	69.336	61.970	13.995	-5.153	-26.746	3.076
2000	9.008	69.798	62.350	14.895	-5.341	-27.883	3.047

Phase change: 1687 K, melting point of Si; ΔH° = 12.082 kcal/mol.

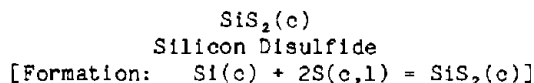
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: Cp° = 8.589 + 0.274x10⁻³T - 0.838x10⁻⁵T²
H° - H°₂₉₈ = 8.589x10⁻³T + 0.137x10⁻⁶T² + 0.838x10⁻²T⁻¹ - 2.854

Reaction equations (kcal/mol):

298.15-1687 K: ΔHr° = 10.538 - 1.262x10⁻³T + 0.374x10⁻⁶T² - 48.850T⁻¹
ΔGr° = 10.538 + 1.262x10⁻³T ln T + 0.374x10⁻⁶T² - 24.425T⁻¹ - 30.656x10⁻³T
1687-2000 K: ΔHr° = -1.891 - 1.683x10⁻³T - 0.023x10⁻⁶T² + 49.650T⁻¹
ΔGr° = -1.891 + 1.683x10⁻³T ln T + 0.023x10⁻⁶T² + 24.825T⁻¹ - 25.842x10⁻³T

Source: Data from Chase (19) who estimated some molecular constants.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	14.730	18.370	18.370	0	-68.600	-68.167	49.967
300*	14.740	18.460	18.370	.030	-68.599	-68.161	49.655
368.3	15.191	21.527	18.689	1.045	-68.693	-68.063	40.388
368.3	15.191	21.527	18.689	1.045	-68.885	-68.063	40.388
388.36	15.323	22.336	18.857	1.351	-68.921	-68.015	38.275
388.36	15.323	22.336	18.857	1.351	-69.747	-68.015	38.275
400	15.400	22.790	18.965	1.530	-69.806	-67.963	37.133
432.02	15.611	23.984	19.293	2.026	-70.007	-67.809	34.303
500	16.060	26.300	20.080	3.110	-70.646	-67.399	29.460
600	16.720	29.290	21.373	4.750	-71.292	-66.688	24.291
700	17.380	31.910	22.696	6.450	-71.783	-65.881	20.569
717.824	17.498	32.348	22.930	6.761	-71.853	-65.728	20.012

*Data above 298 K estimated except temperature of fusion.

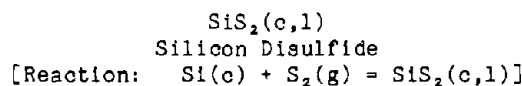
Phase changes: 368.3 K, orthorhombic → monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1363 K: $C_p^\circ = 12.746 + 6.608 \times 10^{-3}T + 0.012 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 12.746 \times 10^{-3}T + 3.304 \times 10^{-6}T^2 - 0.012 \times 10^{-2}T^{-1} - 4.090$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -65.022 - 9.281 \times 10^{-3}T + 6.387 \times 10^{-6}T^2 - 410.900T^{-1}$
 $\Delta G_f^\circ = -65.022 + 9.281 \times 10^{-3}T \ln T - 6.387 \times 10^{-6}T^2 - 205.450T^{-1} - 59.211 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = -67.253 - 4.755 \times 10^{-3}T + 2.895 \times 10^{-6}T^2 - 99.700T^{-1}$
 $\Delta G_f^\circ = -67.253 + 4.755 \times 10^{-3}T \ln T - 2.895 \times 10^{-6}T^2 - 49.850T^{-1} - 28.845 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = -99.569 + 84.725 \times 10^{-3}T - 83.669 \times 10^{-6}T^2 + 3704.700T^{-1}$
 $\Delta G_f^\circ = -99.569 - 84.725 \times 10^{-3}T \ln T + 83.669 \times 10^{-6}T^2 + 1852.350T^{-1} + 541.612 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = -118.527 + 76.913 \times 10^{-3}T - 44.045 \times 10^{-6}T^2 + 10157.700T^{-1}$
 $\Delta G_f^\circ = -118.527 - 76.913 \times 10^{-3}T \ln T + 44.045 \times 10^{-6}T^2 + 5078.850T^{-1} + 537.917 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	14.730	18.370	18.370	0	-99.310	-87.194	63.914
300*	14.740	18.460	18.370	.030	-99.303	-87.116	63.463
400	15.400	22.790	18.965	1.530	-99.108	-83.094	45.400
500	16.060	26.300	20.080	3.110	-98.901	-79.106	34.577
600	16.720	29.290	21.373	4.750	-98.681	-75.169	27.380
700	17.380	31.910	22.696	6.450	-98.433	-71.271	22.251
800	18.040	34.280	24.005	8.220	-98.139	-67.413	18.416
900	18.700	36.440	25.262	10.060	-97.799	-63.588	15.441
1000	19.360	38.440	26.480	11.960	-97.414	-59.797	13.068
1100	20.020	40.320	27.656	13.930	-96.976	-56.067	11.139
1200	20.670	42.090	28.790	15.960	-96.492	-52.374	9.538
1300	21.330	43.770	29.878	18.060	-95.951	-48.719	8.190
1363	21.750	44.780	30.534	19.420	-95.581	-46.422	7.443
1363	23.900	47.770	30.534	23.490	-91.511	-46.422	7.443
1400	23.900	48.410	31.003	24.370	-91.215	-45.208	7.057
1500	23.900	50.060	32.220	26.760	-90.412	-41.964	6.114
1600	23.900	51.600	33.381	29.150	-89.621	-38.757	5.294

*Data above 298 K estimated except temperature of fusion.

Phase change: 1363 K, melting point of SiS₂; ΔH° = 4.07 kcal/mol.

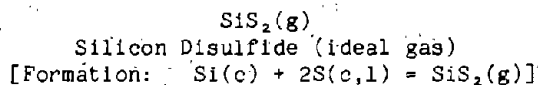
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1363 K: Cp° = 12.746 + 6.608x10⁻³T + 0.012x10⁻⁵T⁻²
H°- H₂₉₈° = 12.746x10⁻³T + 3.304x10⁻⁶T² - 0.012x10⁻²T⁻¹ - 4.090
1363-1600 K: Cp° = 23.900
H°- H₂₉₈° = 23.900x10⁻³T - 9.086

Reaction equations (kcal/mol):

298.15-1363 K: ΔHr° = -98.600 - 1.276x10⁻³T + 2.633x10⁻⁶T² - 168.000T⁻¹
ΔGr° = -98.600 + 1.276x10⁻³TlnT - 2.633x10⁻⁶T² - 84.000T⁻¹ + 32.715x10⁻³T
1363-1600 K: ΔHr° = -103.596 + 9.878x10⁻³T - 0.671x10⁻⁶T² - 166.800T⁻¹
ΔGr° = -103.596 - 9.878x10⁻³TlnT + 0.671x10⁻⁶T² - 83.400T⁻¹ + 112.380x10⁻³T

Source: Data from Gurvich (49) who estimated all above 298 K except temperature of fusion.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	12.384	60.719	60.719	0	1.680	-10.513	7.706
300	12.402	60.796	60.719	.023	1.674	-10.589	7.714
368.3	12.954	63.404	60.981	.892	1.434	-13.359	7.927
368.3	12.954	63.404	60.981	.892	1.242	-13.359	7.927
388.36	13.116	64.095	61.124	1.154	1.161	-14.150	7.963
388.36	13.116	64.095	61.124	1.154	.335	-14.150	7.963
400	13.210	64.484	61.217	1.307	.251	-14.583	7.968
432.02	13.369	65.507	61.497	1.733	-.021	-15.762	7.973
500	13.707	67.490	62.180	2.655	-.821	-18.169	7.942
600	14.022	70.019	63.282	4.042	-1.720	-21.553	7.851
700	14.232	72.197	64.403	5.456	-2.497	-24.796	7.741
717.824	14.258	72.555	64.601	5.710	-2.624	-25.360	7.721

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 14.272 + 0.388x10⁻³T - 1.781x10⁻⁵T²
 H° - H₂₉₈° = 14.272x10⁻³T + 0.194x10⁻⁶T² + 1.781x10⁻²T⁻¹ - 4.870

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 4.478 - 7.755x10⁻³T + 3.277x10⁻⁶T² - 231.600T⁻¹
 ΔGf° = 4.478 + 7.755x10⁻³T ln T - 3.277x10⁻⁶T² - 115.800T⁻¹ - 92.185x10⁻³T
 368.3-388.36 K: ΔHf° = 2.247 - 3.229x10⁻³T - 0.215x10⁻⁶T² + 79.600T⁻¹
 ΔGf° = 2.247 + 3.229x10⁻³T ln T + 0.215x10⁻⁶T² + 39.800T⁻¹ - 61.820x10⁻³T
 388.36-432.02 K: ΔHf° = -30.069 + 86.251x10⁻³T - 86.779x10⁻⁶T² + 3884.000T⁻¹
 ΔGf° = -30.069 - 86.251x10⁻³T ln T + 86.779x10⁻⁶T² + 1942.000T⁻¹ + 508.637x10⁻³T
 432.02-717.824 K: ΔHf° = -49.027 + 78.439x10⁻³T - 47.155x10⁻⁶T² + 10337.000T⁻¹
 ΔGf° = -49.027 - 78.439x10⁻³T ln T + 47.155x10⁻⁶T² + 5168.500T⁻¹ + 504.942x10⁻³T

$\text{SiS}_2(\text{g})$
 Silicon Disulfide (ideal gas)
 [Reaction: $\text{Si}(\text{c}, \text{l}) + \text{S}_2(\text{g}) = \text{SiS}_2(\text{g})$]

T, K	cal/mol·K						Log Kr
	C_p°	S°	$-(C_p^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	12.384	60.719	60.719	0	-29.100	-29.541	21.654
300	12.402	60.796	60.719	.023	-29.099	-29.543	21.522
400	13.210	64.484	61.217	1.307	-29.091	-29.715	16.235
500	13.707	67.490	62.180	2.655	-29.074	-29.875	13.058
600	14.022	70.019	63.282	4.042	-29.109	-30.035	10.940
700	14.232	72.197	64.403	5.456	-29.147	-30.186	9.424
800	14.377	74.108	65.501	6.886	-29.193	-30.330	8.286
900	14.480	75.807	66.551	8.330	-29.249	-30.468	7.399
1000	14.556	77.337	67.555	9.782	-29.312	-30.592	6.686
1100	14.614	78.727	68.509	11.240	-29.386	-30.725	6.104
1200	14.658	80.001	69.414	12.704	-29.468	-30.843	5.617
1300	14.694	81.175	70.273	14.172	-29.559	-30.954	5.204
1400	14.722	82.265	71.092	15.642	-29.663	-31.053	4.848
1500	14.745	83.282	71.871	17.116	-29.776	-31.160	4.540
1600	14.764	84.234	72.615	18.591	-29.900	-31.250	4.269
1687	14.777	85.017	73.234	19.877	-30.017	-31.301	4.055
1687	14.777	85.017	73.234	19.877	-42.099	-31.301	4.055
1700	14.779	85.130	73.325	20.069	-42.108	-31.213	4.013
1800	14.793	85.975	74.004	21.547	-42.184	-30.567	3.711
1900	14.804	86.775	74.656	23.027	-42.265	-29.919	3.441
2000	14.813	87.534	75.280	24.508	-42.351	-29.271	3.199

Phase change: 1687 K, melting point of Si; $\Delta H^\circ = 12.082$ kcal/mol.

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

298.15-2000 K: $C_p^\circ = 14.272 + 0.388 \times 10^{-3}T - 1.781 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 14.272 \times 10^{-3}T + 0.194 \times 10^{-6}T^2 + 1.781 \times 10^{-2}T^3 - 4.870$

Reaction equations (kcal/mol):

298.15-1687 K: $\Delta H_r^\circ = -29.100 + 0.250 \times 10^{-3}T - 0.477 \times 10^{-6}T^2 + 11.300T^{-1}$
 $\Delta G_r^\circ = -29.100 - 0.250 \times 10^{-3}T \ln T + 0.477 \times 10^{-6}T^2 + 5.650T^{-1} - 0.259 \times 10^{-3}T$
 1687-2000 K: $\Delta H_r^\circ = -41.529 - 0.171 \times 10^{-3}T - 0.126 \times 10^{-6}T^2 + 109.800T^{-1}$
 $\Delta G_r^\circ = -41.529 + 0.171 \times 10^{-3}T \ln T + 0.126 \times 10^{-6}T^2 + 54.900T^{-1} + 4.555 \times 10^{-3}T$

Source: Data from Gurvich (49).

SmS(g)
Samarium Monosulfide (ideal gas)
[Formation: $\text{Sm}(c) + \text{S}(c,l) = \text{SmS}(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15*	8.200	63.970	63.970	0	22.100	10.270	-7.528
300	8.210	64.020	63.970	.015	22.092	10.195	-7.427
368.3	8.415	65.731	64.144	.585	21.779	7.519	-4.462
368.3	8.415	65.731	64.144	.585	21.683	7.519	-4.462
388.36	8.475	66.179	64.237	.754	21.578	6.751	-3.799
388.36	8.475	66.179	64.237	.754	21.165	6.751	-3.799
400	8.510	66.430	64.298	.853	21.084	6.320	-3.453
432.02	8.555	67.087	64.480	1.126	20.835	5.147	-2.604
500	8.650	68.340	64.916	1.712	20.160	2.739	-1.197
600	8.730	69.930	65.628	2.581	19.235	-.666	.243
700	8.780	71.280	66.343	3.456	18.308	-3.906	1.219
717.824	8.785	71.501	66.468	3.613	18.145	-4.469	1.361

*Data except enthalpy of formation at 298 K estimated.

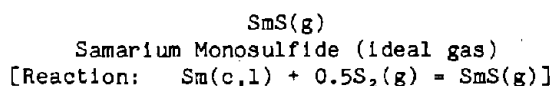
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: $C_p^\circ = 8.875 + 0.036 \times 10^{-3}T - 0.608 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 8.875 \times 10^{-3}T + 0.018 \times 10^{-6}T^2 + 0.608 \times 10^{-2}T^{-1} - 2.852$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 25.235 - 7.499 \times 10^{-3}T + 0.250 \times 10^{-6}T^2 - 274.800T^{-1}$
 $\Delta G_f^\circ = 25.235 + 7.499 \times 10^{-3}T \ln T - 0.250 \times 10^{-6}T^2 - 137.400T^{-1} - 91.301 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = 24.120 - 5.236 \times 10^{-3}T - 1.496 \times 10^{-6}T^2 - 119.200T^{-1}$
 $\Delta G_f^\circ = 24.120 + 5.236 \times 10^{-3}T \ln T + 1.496 \times 10^{-6}T^2 - 59.600T^{-1} - 76.118 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = 7.962 + 39.504 \times 10^{-3}T - 44.778 \times 10^{-6}T^2 + 1783.000T^{-1}$
 $\Delta G_f^\circ = 7.962 - 39.504 \times 10^{-3}T \ln T + 44.778 \times 10^{-6}T^2 + 891.500T^{-1} + 209.110 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = -1.517 + 35.598 \times 10^{-3}T - 24.966 \times 10^{-6}T^2 + 5009.500T^{-1}$
 $\Delta G_f^\circ = -1.517 - 35.598 \times 10^{-3}T \ln T + 24.966 \times 10^{-6}T^2 + 2504.750T^{-1} + 207.263 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	8.200	63.970	63.970	0	6.745	.756	-.554
300	8.210	64.020	63.970	.015	6.740	.718	-.523
400	8.510	66.430	64.298	.853	6.433	-1.246	.681
500	8.650	68.340	64.916	1.712	6.033	-3.115	1.361
600	8.730	69.930	65.628	2.581	5.541	-4.907	1.787
700	8.780	71.280	66.343	3.456	4.983	-6.601	2.061
800	8.810	72.450	67.031	4.335	4.394	-8.212	2.243
900	8.830	73.490	67.693	5.217	3.774	-9.753	2.368
1000	8.850	74.420	68.318	6.102	3.144	-11.217	2.452
1100	8.860	75.270	68.918	6.987	2.482	-12.638	2.511
1190	8.878	75.966	69.424	7.785	1.853	-13.848	2.543
1190	8.878	75.966	69.424	7.785	1.109	-13.848	2.543
1200	8.880	76.040	69.478	7.874	1.041	-13.962	2.543
1300	8.880	76.750	70.010	8.762	.352	-15.195	2.554
1345	8.885	77.052	70.241	9.162	.041	-15.718	2.554
1345	8.885	77.052	70.241	9.162	-2.019	-15.718	2.554
1400	8.890	77.410	70.516	9.651	-2.442	-16.273	2.540
1500	8.900	78.020	70.993	10.541	-3.214	-17.225	2.510
1600	8.910	78.600	71.455	11.432	-3.989	-18.149	2.479
1700	8.910	79.140	71.891	12.323	-4.768	-19.006	2.443
1800	8.920	79.650	72.309	13.214	-5.549	-19.832	2.408
1900	8.930	80.130	72.705	14.107	-6.331	-20.597	2.369
2000	8.930	80.590	73.090	15.000	-7.116	-21.322	2.330

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1190 K, α - β transition point of Sm; ΔH° = 0.744 kcal/mol.
1345 K, melting point of Sm; ΔH° = 2.060 kcal/mol.

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

298.15-2000 K: $\text{Cp}^\circ = 8.875 + 0.036 \times 10^{-3}T - 0.608 \times 10^{-5}T^{-2}$
 $\text{H}^\circ - \text{H}_{298}^\circ = 8.875 \times 10^{-3}T + 0.018 \times 10^{-6}T^2 + 0.608 \times 10^{-2}T^{-1} - 2.852$

Reaction equations (kcal/mol):

298.15-1190 K: $\Delta \text{Hr}^\circ = 8.446 - 3.496 \times 10^{-3}T - 1.627 \times 10^{-6}T^2 - 153.350T^{-1}$
 $\Delta \text{Gr}^\circ = 8.446 + 3.496 \times 10^{-3}T \ln T + 1.627 \times 10^{-6}T^2 - 76.675T^{-1} - 45.338 \times 10^{-3}T$
1190-1345 K: $\Delta \text{Hr}^\circ = 9.042 - 6.517 \times 10^{-3}T - 0.142 \times 10^{-6}T^2 + 26.650T^{-1}$
 $\Delta \text{Gr}^\circ = 9.042 + 6.517 \times 10^{-3}T \ln T + 0.142 \times 10^{-6}T^2 + 13.325T^{-1} - 65.522 \times 10^{-3}T$
1345-2000 K: $\Delta \text{Hr}^\circ = 8.031 - 7.296 \times 10^{-3}T - 0.142 \times 10^{-6}T^2 + 26.650T^{-1}$
 $\Delta \text{Gr}^\circ = 8.031 + 7.296 \times 10^{-3}T \ln T + 0.142 \times 10^{-6}T^2 + 13.325T^{-1} - 70.389 \times 10^{-3}T$

Source: Data from Mills (80) who estimated all except enthalpy of formation at 298 K.

SnS(c)
Tin Monosulfide
[Formation: $\text{Sn}(\beta, l) + \text{S}(c, l) = \text{SnS}(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	11.770	18.400	18.400	0	-26.000	-25.554	18.731
300	11.780	18.470	18.403	.020	-26.002	-25.552	18.614
368.3	12.067	20.918	18.650	.835	-26.021	-25.447	15.100
368.3	12.067	20.918	18.650	.835	-26.117	-25.447	15.100
388.36	12.151	21.560	18.784	1.078	-26.130	-25.410	14.299
388.36	12.151	21.560	18.784	1.078	-26.543	-25.410	14.299
400	12.200	21.920	18.870	1.220	-26.569	-25.376	13.865
432.02	12.315	22.864	19.131	1.612	-26.662	-25.277	12.787
500	12.560	24.680	19.760	2.460	-26.977	-25.030	10.940
505.12	12.588	24.808	19.811	2.524	-26.997	-25.011	10.821
505.12	12.588	24.808	19.811	2.524	-28.677	-25.011	10.821
600	13.100	27.020	20.787	3.740	-28.928	-24.298	8.851
700	13.900	29.090	21.819	5.090	-29.062	-23.507	7.339
717.824	14.092	29.442	22.003	5.339	-29.071	-23.365	7.114

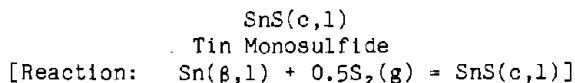
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 505.12 K, melting point of Sn; $\Delta H^\circ = 1.680$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-875 K: $C_p^\circ = 8.066 + 8.254 \times 10^{-3}T + 1.105 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 8.066 \times 10^{-3}T + 4.127 \times 10^{-6}T^2 - 1.105 \times 10^{-2}T^{-1} - 2.401$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -23.931 - 5.076 \times 10^{-3}T + 3.502 \times 10^{-6}T^2 - 258.500T^{-1}$
 $\Delta G_f^\circ = -23.931 + 5.076 \times 10^{-3}T \ln T - 3.502 \times 10^{-6}T^2 - 129.250T^{-1} - 31.866 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -25.046 - 2.813 \times 10^{-3}T + 1.756 \times 10^{-6}T^2 - 102.900T^{-1}$
 $\Delta G_f^\circ = -25.046 + 2.813 \times 10^{-3}T \ln T - 1.756 \times 10^{-6}T^2 - 51.450T^{-1} - 16.683 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -41.204 + 41.927 \times 10^{-3}T - 41.526 \times 10^{-6}T^2 + 1799.300T^{-1}$
 $\Delta G_f^\circ = -41.204 - 41.927 \times 10^{-3}T \ln T + 41.526 \times 10^{-6}T^2 + 899.650T^{-1} + 268.546 \times 10^{-3}T$
 432.02-505.12 K: $\Delta H_f^\circ = -50.683 + 38.021 \times 10^{-3}T - 21.714 \times 10^{-6}T^2 + 5025.800T^{-1}$
 $\Delta G_f^\circ = -50.683 - 38.021 \times 10^{-3}T \ln T + 21.714 \times 10^{-6}T^2 + 2512.900T^{-1} + 266.698 \times 10^{-3}T$
 505.12-717.824 K: $\Delta H_f^\circ = -52.649 + 36.798 \times 10^{-3}T - 19.553 \times 10^{-6}T^2 + 5203.600T^{-1}$
 $\Delta G_f^\circ = -52.649 - 36.798 \times 10^{-3}T \ln T + 19.553 \times 10^{-6}T^2 + 2601.800T^{-1} + 263.720 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	11.770	18.400	18.400	0	-41.355	-35.067	25.705
300	11.780	18.470	18.403	.020	-41.354	-35.029	25.518
400	12.200	21.920	18.870	1.220	-41.220	-32.941	17.998
500	12.560	24.680	19.760	2.460	-41.104	-30.883	13.499
505.12	12.588	24.808	19.811	2.524	-41.100	-30.779	13.317
505.12	12.588	24.808	19.811	2.524	-42.780	-30.779	13.317
600	13.100	27.020	20.787	3.740	-42.623	-28.539	10.395
700	13.900	29.090	21.819	5.090	-42.387	-26.203	8.181
800	14.980	31.020	22.858	6.530	-42.063	-23.918	6.534
875	15.990	32.400	23.613	7.690	-41.742	-22.228	5.552
875	12.920	32.540	23.613	7.810	-41.622	-22.228	5.552
900	13.050	32.910	23.877	8.130	-41.583	-21.684	5.266
1000	13.560	34.310	24.850	9.460	-41.376	-19.484	4.258
1100	14.070	35.620	25.756	10.850	-41.114	-17.291	3.435
1153	14.350	36.290	26.229	11.600	-40.962	-16.151	3.061
1153	18.000	42.820	26.229	19.130	-33.432	-16.151	3.061
1200	18.000	43.540	26.890	19.980	-33.115	-15.449	2.814
1300	18.000	44.980	28.226	21.780	-32.449	-14.003	2.354

Phase changes: 505.12 K, melting point of Sn; ΔH° = 1.680 kcal/mol.
875 K, α - β transition point of SnS; ΔH° = 0.120 kcal/mol.
1153 K, melting point of SnS; ΔH° = 7.530 kcal/mol.

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

298.15-875 K: $C_p^\circ = 8.066 + 8.254 \times 10^{-3}T + 1.105 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 8.066 \times 10^{-3}T + 4.127 \times 10^{-6}T^2 - 1.105 \times 10^{-2}T^{-1} - 2.401$
 875-1153 K: $C_p^\circ = 8.429 + 5.132 \times 10^{-3}T$
 $H^\circ - H_{298}^\circ = 8.429 \times 10^{-3}T + 2.566 \times 10^{-6}T^2 - 1.530$
 1153-1300 K: $C_p^\circ = 18.000$
 $H^\circ - H_{298}^\circ = 18.000 \times 10^{-3}T - 1.624$

Reaction equations (kcal/mol):

298.15-505.12 K: $\Delta H_r^\circ = -40.720 - 1.074 \times 10^{-3}T + 1.625 \times 10^{-6}T^2 - 137.050T^{-1}$
 $\Delta G_r^\circ = -40.720 + 1.074 \times 10^{-3}T \ln T - 1.625 \times 10^{-6}T^2 - 68.525T^{-1} + 14.097 \times 10^{-3}T$
 505.12-875 K: $\Delta H_r^\circ = -42.685 - 2.296 \times 10^{-3}T + 3.786 \times 10^{-6}T^2 + 40.750T^{-1}$
 $\Delta G_r^\circ = -42.685 + 2.296 \times 10^{-3}T \ln T - 3.786 \times 10^{-6}T^2 + 20.375T^{-1} + 11.119 \times 10^{-3}T$
 875-1153 K: $\Delta H_r^\circ = -41.814 - 1.934 \times 10^{-3}T + 2.225 \times 10^{-6}T^2 + 151.250T^{-1}$
 $\Delta G_r^\circ = -41.814 + 1.934 \times 10^{-3}T \ln T - 2.225 \times 10^{-6}T^2 + 75.625T^{-1} + 11.144 \times 10^{-3}T$
 1153-1300 K: $\Delta H_r^\circ = -41.908 + 7.637 \times 10^{-3}T - 0.341 \times 10^{-6}T^2 + 151.250T^{-1}$
 $\Delta G_r^\circ = -41.908 - 7.637 \times 10^{-3}T \ln T + 0.341 \times 10^{-6}T^2 + 75.625T^{-1} + 75.744 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mills (80). Low-temperature heat capacities and entropy at 298 K from King (65). High-temperature data based on Orr (89).

SnS(g)
Tin Monosulfide (ideal gas)
[Formation: $\text{Sn}(s, l) + \text{S}(c, l) = \text{SnS}(g)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	8.230	57.900	57.900	0	26.700	15.369	-11.266
300	8.240	57.950	57.900	.015	26.693	15.299	-11.145
368.3	8.431	59.670	58.076	.587	26.431	12.732	-7.555
368.3	8.431	59.670	58.076	.587	26.335	12.732	-7.555
388.36	8.487	60.119	58.170	.757	26.249	11.994	-6.750
388.36	8.487	60.119	58.170	.757	25.836	11.994	-6.750
400	8.520	60.370	58.230	.856	25.767	11.580	-6.327
432.02	8.562	61.028	58.413	1.129	25.555	10.452	-5.287
500	8.650	62.290	58.860	1.715	24.978	8.121	-3.549
505.12	8.654	62.378	58.895	1.759	24.938	7.947	-3.438
505.12	8.654	62.378	58.895	1.759	23.258	7.947	-3.438
600	8.730	63.870	59.563	2.584	22.616	5.136	-1.871
700	8.770	65.220	60.279	3.459	22.007	2.271	-.709
717.824	8.777	65.441	60.404	3.615	21.905	1.770	-.539

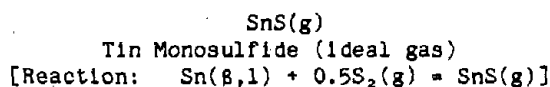
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 505.12 K, melting point of Sn; $\Delta H^\circ = 1.680$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: $C_p^\circ = 8.838 + 0.074 \times 10^{-3}T - 0.560 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 8.838 \times 10^{-3}T + 0.037 \times 10^{-6}T^2 + 0.560 \times 10^{-2}T^{-1} - 2.826$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 28.344 - 4.304 \times 10^{-3}T - 0.588 \times 10^{-6}T^2 - 92.000T^{-1}$
 $\Delta G_f^\circ = 28.344 + 4.304 \times 10^{-3}T \ln T + 0.588 \times 10^{-6}T^2 - 46.000T^{-1} - 67.698 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = 27.229 - 2.041 \times 10^{-3}T - 2.334 \times 10^{-6}T^2 + 63.600T^{-1}$
 $\Delta G_f^\circ = 27.229 + 2.041 \times 10^{-3}T \ln T + 2.334 \times 10^{-6}T^2 + 31.800T^{-1} - 52.515 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = 11.071 + 42.699 \times 10^{-3}T - 45.616 \times 10^{-6}T^2 + 1965.800T^{-1}$
 $\Delta G_f^\circ = 11.071 - 42.699 \times 10^{-3}T \ln T + 45.616 \times 10^{-6}T^2 + 982.900T^{-1} + 232.714 \times 10^{-3}T$
 432.02-505.12 K: $\Delta H_f^\circ = 1.592 + 38.793 \times 10^{-3}T - 25.804 \times 10^{-6}T^2 + 5192.300T^{-1}$
 $\Delta G_f^\circ = 1.592 - 38.793 \times 10^{-3}T \ln T + 25.804 \times 10^{-6}T^2 + 2596.150T^{-1} + 230.866 \times 10^{-3}T$
 505.12-717.82 K: $\Delta H_f^\circ = -0.374 + 37.570 \times 10^{-3}T - 23.643 \times 10^{-6}T^2 + 5370.100T^{-1}$
 $\Delta G_f^\circ = -0.374 - 37.570 \times 10^{-3}T \ln T + 23.643 \times 10^{-6}T^2 + 2685.050T^{-1} + 227.888 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{f,298}^\circ)/T$	$H^\circ - H_{f,298}^\circ$	ΔH_r°	ΔG_r°	
298.15	8.230	57.900	57.900	0	11.345	5.856	-4.292
300	8.240	57.950	57.900	.015	11.341	5.822	-4.241
400	8.520	60.370	58.230	.856	11.116	4.015	-2.193
500	8.650	62.290	58.860	1.715	10.851	2.267	-.991
505.12	8.654	62.378	58.895	1.759	10.835	2.178	-.942
505.12	8.654	62.378	58.895	1.759	9.155	2.178	-.942
600	8.730	63.870	59.563	2.584	8.922	.895	-.326
700	8.770	65.220	60.279	3.459	8.682	-.425	.133
800	8.810	66.390	60.967	4.338	8.445	-1.706	.466
900	8.830	67.430	61.629	5.221	8.209	-2.961	.719
1000	8.860	68.360	62.255	6.105	7.969	-4.189	.915
1100	8.870	69.210	62.855	6.991	7.728	-5.399	1.073
1200	8.890	69.980	63.414	7.879	7.485	-6.578	1.198
1300	8.900	70.690	63.945	8.769	7.240	-7.737	1.301
1400	8.910	71.350	64.450	9.660	6.993	-8.878	1.386
1500	8.930	71.970	64.935	10.552	6.743	-10.010	1.458
1600	8.940	72.550	65.397	11.445	6.490	-11.126	1.520
1700	8.950	73.090	65.832	12.339	6.235	-12.216	1.571
1800	8.960	73.600	66.248	13.234	5.978	-13.291	1.614
1900	8.970	74.080	66.643	14.130	5.718	-14.345	1.650
2000	8.980	74.540	67.026	15.028	5.458	-15.395	1.682

Phase change: 505.12 K, melting point of Sn; $\Delta H^\circ = 1.680$ kcal/mol.

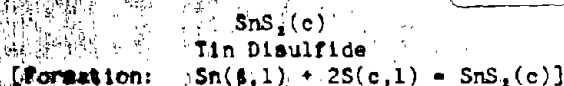
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 8.838 + 0.074 \times 10^{-3}T - 0.560 \times 10^{-5}T^{-2}$
 $H^\circ - H_{f,298}^\circ = 8.838 \times 10^{-3}T + 0.037 \times 10^{-6}T^2 + 0.560 \times 10^{-2}T^{-1} - 2.826$

Reaction equations (kcal/mol):

298.15-505.12 K: $\Delta H_r^\circ = 11.555 - 0.301 \times 10^{-3}T - 2.465 \times 10^{-6}T^2 + 29.450T^{-1}$
 $\Delta G_r^\circ = 11.555 + 0.301 \times 10^{-3}T \ln T + 2.465 \times 10^{-6}T^2 + 14.725T^{-1} - 21.735 \times 10^{-3}T$
505.12-2000 K: $\Delta H_r^\circ = 9.590 - 1.524 \times 10^{-3}T - 0.304 \times 10^{-6}T^2 + 207.250T^{-1}$
 $\Delta G_r^\circ = 9.590 + 1.524 \times 10^{-3}T \ln T + 0.304 \times 10^{-6}T^2 + 103.625T^{-1} - 24.713 \times 10^{-3}T$

Source: Data from Mills (80).



T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{f,0}^\circ)/T$	$H^\circ - H_{f,0}^\circ$	ΔH_f°	ΔG_f°	
298.15	16.470	20.930	20.930	0	-35.800	-33.824	24.793
300	16.490	21.040	20.940	.030	-35.802	-33.814	24.633
368.3	17.030	24.494	21.300	1.176	-35.875	-33.359	19.795
368.3	17.030	24.494	21.300	1.176	-36.067	-33.359	19.795
388.36	17.188	25.401	21.489	1.519	-36.098	-33.210	18.689
388.36	17.188	25.401	21.489	1.519	-36.924	-33.210	18.689
400	17.280	25.910	21.610	1.720	-36.979	-33.098	18.084
432.02	17.424	27.246	21.979	2.276	-37.172	-32.781	16.583
500	17.730	29.800	22.840	3.480	-37.804	-32.018	13.995
505.12	17.748	29.981	22.911	3.571	-37.844	-31.960	13.828
505.12	17.748	29.981	22.911	3.571	-39.524	-31.960	13.828
600	18.090	33.080	24.297	5.270	-40.102	-30.491	11.106
700	18.450	35.900	25.771	7.090	-40.566	-28.861	9.011
717.824	18.519	36.365	26.029	7.419	-40.632	-28.561	8.696

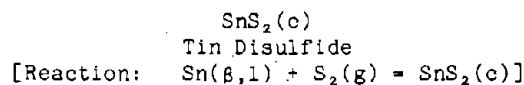
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 505.12 K, melting point of Sn; $\Delta H^\circ = 1.680$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-1000. K: $C_p^\circ = 17.157 + 2.228 \times 10^{-3}T + 1.202 \times 10^{-5}T^2$
 $H^\circ - H_{f,0}^\circ = 17.157 \times 10^{-3}T + 1.114 \times 10^{-6}T^2 + 1.202 \times 10^{-2}T^3 - 5.618$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -34.141 - 4.159 \times 10^{-3}T + 2.206 \times 10^{-5}T^2 - 183.400T^{-1}$
 $\Delta G_f^\circ = -34.141 + 4.159 \times 10^{-3}T \ln T - 2.206 \times 10^{-5}T^2 - 91.700T^{-1} - 20.943 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -36.371 + 0.367 \times 10^{-3}T - 1.286 \times 10^{-5}T^2 + 127.800T^{-1}$
 $\Delta G_f^\circ = -36.371 - 0.367 \times 10^{-3}T \ln T + 1.286 \times 10^{-5}T^2 + 63.900T^{-1} + 9.422 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -68.688 + 89.847 \times 10^{-3}T - 87.850 \times 10^{-6}T^2 + 3932.200T^{-1}$
 $\Delta G_f^\circ = -68.688 - 89.847 \times 10^{-3}T \ln T + 87.850 \times 10^{-6}T^2 + 1966.100T^{-1} + 579.879 \times 10^{-3}T$
 432.02-505.12 K: $\Delta H_f^\circ = -87.645 + 82.035 \times 10^{-3}T - 48.226 \times 10^{-6}T^2 + 10385.200T^{-1}$
 $\Delta G_f^\circ = -87.645 - 82.035 \times 10^{-3}T \ln T + 48.226 \times 10^{-6}T^2 + 5192.600T^{-1} + 576.184 \times 10^{-3}T$
 505.12-717.824 K: $\Delta H_f^\circ = -89.611 + 80.812 \times 10^{-3}T - 46.065 \times 10^{-6}T^2 + 10563.000T^{-1}$
 $\Delta G_f^\circ = -89.611 - 80.812 \times 10^{-3}T \ln T + 46.065 \times 10^{-6}T^2 + 5281.500T^{-1} + 573.206 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHr°	ΔGr°	
298.15	16.470	20.930	20.930	0	-66.510	-52.851	38.740
300	16.490	21.040	20.940	.030	-66.506	-52.769	38.441
400	17.280	25.910	21.610	1.720	-66.281	-48.229	26.351
500	17.730	29.800	22.840	3.480	-66.059	-43.724	19.112
505.12	17.748	29.981	22.911	3.571	-66.049	-43.497	18.820
505.12	17.748	29.981	22.911	3.571	-67.729	-43.497	18.820
600	18.090	33.080	24.297	5.270	-67.491	-38.973	14.196
700	18.450	35.900	25.771	7.090	-67.216	-34.252	10.694
800	18.840	38.380	27.180	8.960	-66.897	-29.550	8.073
900	19.270	40.630	28.563	10.860	-66.557	-24.914	6.050
1000	19.750	42.690	29.880	12.810	-66.174	-20.313	4.439

Phase change: 505.12 K, melting point of Sn; $\Delta\text{H}^\circ = 1.680$ kcal/mol.

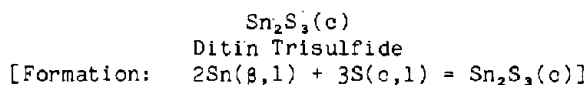
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1000 K: $\text{Cp}^\circ = 17.157 + 2.228 \times 10^{-3} \text{T} - 1.202 \times 10^{-5} \text{T}^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 17.157 \times 10^{-3} \text{T} + 1.114 \times 10^{-6} \text{T}^2 + 1.202 \times 10^{-2} \text{T}^{-1} - 5.618$

Reaction equations (kcal/mol):

298.15-505.12 K: $\Delta\text{Hr}^\circ = -67.719 + 3.846 \times 10^{-3} \text{T} - 1.548 \times 10^{-6} \text{T}^2 + 59.500 \text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -67.719 - 3.846 \times 10^{-3} \text{T} \ln \text{T} + 1.548 \times 10^{-6} \text{T}^2 + 29.750 \text{T}^{-1} + 70.983 \times 10^{-3} \text{T}$
 505.12-1000 K: $\Delta\text{Hr}^\circ = -69.684 + 2.623 \times 10^{-3} \text{T} + 0.613 \times 10^{-6} \text{T}^2 + 237.300 \text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -69.684 - 2.623 \times 10^{-3} \text{T} \ln \text{T} - 0.613 \times 10^{-6} \text{T}^2 + 118.650 \text{T}^{-1} + 68.004 \times 10^{-3} \text{T}$

Sources: Enthalpy of formation at 298 K from Wiedemeier (129). Other data from Wiedemeier (131).



T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	28.320	39.100	39.100	0	-60.800	-58.309	42.741
300	28.350	39.290	39.123	.050	-60.804	-58.300	42.471
368.3	29.197	45.203	39.696	2.028	-60.879	-57.714	34.247
368.3	29.197	45.203	39.696	2.028	-61.167	-57.714	34.247
388.36	29.446	46.758	40.021	2.616	-61.209	-57.522	32.370
388.36	29.446	46.758	40.021	2.616	-62.448	-57.522	32.370
400	29.590	47.630	40.230	2.960	-62.528	-57.374	31.347
432.02	29.821	49.918	40.864	3.911	-62.812	-56.952	28.811
500	30.310	54.330	42.430	5.950	-63.771	-55.963	24.461
505.12	30.340	54.639	42.552	6.105	-63.831	-55.885	24.179
505.12	30.340	54.639	42.552	6.105	-67.191	-55.885	24.179
600	30.900	59.890	44.873	9.010	-68.030	-53.664	19.547
650	31.190	62.380	46.118	10.570	-68.370	-52.447	17.634

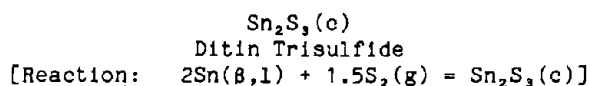
Phase changes: 368.3 K, orthorhombic $\rightarrow$ monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 505.12 K, melting point of Sn; $\Delta H^\circ = 1.680$ kcal/mol.

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

298.15-650 K: $C_p^\circ = 28.900 + 4.172 \times 10^{-3}T - 1.621 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 28.900 \times 10^{-3}T + 2.086 \times 10^{-6}T^2 + 1.621 \times 10^{-2}T^3 - 9.346$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -58.399 - 5.558 \times 10^{-3}T + 2.553 \times 10^{-6}T^2 - 289.500T^{-1}$
 $\Delta G_f^\circ = -58.399 + 5.558 \times 10^{-3}T \ln T - 2.553 \times 10^{-6}T^2 - 144.750T^{-1} - 28.976 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -61.744 + 1.231 \times 10^{-3}T - 2.685 \times 10^{-6}T^2 + 177.300T^{-1}$
 $\Delta G_f^\circ = -61.744 - 1.231 \times 10^{-3}T \ln T + 2.685 \times 10^{-6}T^2 + 88.650T^{-1} + 16.573 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -110.219 + 135.451 \times 10^{-3}T - 132.531 \times 10^{-6}T^2 + 5883.900T^{-1}$
 $\Delta G_f^\circ = -110.219 - 135.451 \times 10^{-3}T \ln T + 132.531 \times 10^{-6}T^2 + 2941.950T^{-1} + 872.258 \times 10^{-3}T$
 432.02-505.12 K: $\Delta H_f^\circ = -138.655 + 123.733 \times 10^{-3}T - 73.095 \times 10^{-6}T^2 + 15563.400T^{-1}$
 $\Delta G_f^\circ = -138.655 - 123.733 \times 10^{-3}T \ln T + 73.095 \times 10^{-6}T^2 + 7781.700T^{-1} + 866.715 \times 10^{-3}T$
 505.12-650 K: $\Delta H_f^\circ = -142.586 + 121.287 \times 10^{-3}T - 68.773 \times 10^{-6}T^2 + 15919.000T^{-1}$
 $\Delta G_f^\circ = -142.586 - 121.287 \times 10^{-3}T \ln T + 68.773 \times 10^{-6}T^2 + 7959.500T^{-1} + 860.758 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHr°	ΔGr°	
298.15	28.320	39.100	39.100	0	-106.865	-86.850	63.662
300	28.350	39.290	39.123	.050	-106.860	-86.732	63.183
400	29.590	47.630	40.230	2.960	-106.481	-80.071	43.748
500	30.310	54.330	42.430	5.950	-106.153	-73.522	32.136
505.12	30.340	54.639	42.552	6.105	-106.139	-73.191	31.667
505.12	30.340	54.639	42.552	6.105	-109.499	-73.191	31.667
600	30.900	59.890	44.873	9.010	-109.114	-66.386	24.181
650	31.190	62.380	46.118	10.570	-108.882	-62.830	21.125

Phase change: 505.12 K, melting point of Sn; $\Delta\text{H}^\circ = 1.680$ kcal/mol.

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

298.15-650 K: $\text{Cp}^\circ = 28.900 + 4.172 \times 10^{-3}\text{T} - 1.621 \times 10^{-5}\text{T}^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 28.900 \times 10^{-3}\text{T} + 2.086 \times 10^{-6}\text{T}^2 + 1.621 \times 10^{-2}\text{T}^{-1} - 9.346$

Reaction equations (kcal/mol):

298.15-505.12 K: $\Delta\text{Hr}^\circ = -108.765 + 6.449 \times 10^{-3}\text{T} - 3.078 \times 10^{-6}\text{T}^2 + 74.850\text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -108.765 - 6.449 \times 10^{-3}\text{T} \ln \text{T} + 3.078 \times 10^{-6}\text{T}^2 + 37.425\text{T}^{-1} + 108.913 \times 10^{-3}\text{T}$
 505.12-650 K: $\Delta\text{Hr}^\circ = -112.697 + 4.003 \times 10^{-3}\text{T} + 1.244 \times 10^{-6}\text{T}^2 + 430.450\text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -112.697 - 4.003 \times 10^{-3}\text{T} \ln \text{T} - 1.244 \times 10^{-6}\text{T}^2 + 215.225\text{T}^{-1} + 102.956 \times 10^{-3}\text{T}$

Sources: Enthalpy of formation at 298 K from Wiedemeier (130). Other data from Wiedemeier (131) who extrapolated heat capacities 0-110 K to derive entropy at 298 K.

SrS(c)
Strontium Sulfide
[Formation: $\text{Sr(c)} + \text{S(c,l)} = \text{SrS(c)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H _{2,98} °)/T	H°- H _{2,98} °	ΔHf°	ΔGf°	
298.15	11.640	16.350	16.350	0	-112.000	-110.864	81.264
300*	11.646	16.422	16.350	.022	-112.000	-110.856	80.758
368.3	11.888	18.834	16.595	.824	-112.027	-110.594	65.626
368.3	11.888	18.834	16.595	.824	-112.123	-110.594	65.626
388.36	11.959	19.466	16.728	1.064	-112.138	-110.510	62.189
388.36	11.959	19.466	16.728	1.064	-112.551	-110.510	62.189
400	12.000	19.820	16.813	1.203	-112.578	-110.449	60.346
432.02	12.128	20.749	17.070	1.589	-112.674	-110.275	55.785
500	12.400	22.543	17.695	2.424	-112.993	-109.870	48.024
600	12.710	24.832	18.699	3.680	-113.336	-109.212	39.780
700	12.930	26.808	19.718	4.963	-113.644	-108.500	33.875
717.824	12.964	27.133	19.898	5.194	-113.697	-108.368	32.994

*Data above 298 K estimated.

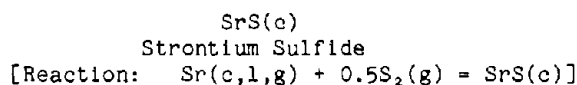
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: $C_p^\circ = 12.021 + 1.416 \times 10^{-3}T - 0.714 \times 10^{-5}T^2$
 $H^\circ - H_{2,98}^\circ = 12.021 \times 10^{-3}T + 0.708 \times 10^{-6}T^2 + 0.714 \times 10^{-2}T^{-1} - 3.886$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -111.572 - 0.747 \times 10^{-3}T - 0.107 \times 10^{-6}T^2 - 58.500T^{-1}$
 $\Delta G_f^\circ = -111.572 + 0.747 \times 10^{-3}T \ln T + 0.107 \times 10^{-6}T^2 - 29.250T^{-1} - 1.585 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = -112.687 + 1.516 \times 10^{-3}T - 1.853 \times 10^{-6}T^2 + 97.100T^{-1}$
 $\Delta G_f^\circ = -112.687 - 1.516 \times 10^{-3}T \ln T + 1.853 \times 10^{-6}T^2 + 48.550T^{-1} + 13.598 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = -128.845 + 46.256 \times 10^{-3}T - 45.135 \times 10^{-6}T^2 + 1999.300T^{-1}$
 $\Delta G_f^\circ = -128.845 - 46.256 \times 10^{-3}T \ln T + 45.135 \times 10^{-6}T^2 + 999.650T^{-1} + 298.826 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = -138.324 + 42.350 \times 10^{-3}T - 25.323 \times 10^{-6}T^2 + 5225.800T^{-1}$
 $\Delta G_f^\circ = -138.324 - 42.350 \times 10^{-3}T \ln T + 25.323 \times 10^{-6}T^2 + 2612.900T^{-1} + 296.979 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	11.640	16.350	16.350	0	-127.355	-120.377	88.238
300*	11.646	16.422	16.350	.022	-127.352	-120.333	87.662
400	12.000	19.820	16.813	1.203	-127.229	-118.014	64.479
500	12.400	22.543	17.695	2.424	-127.120	-115.723	50.582
600	12.710	24.832	18.699	3.680	-127.031	-113.453	41.325
700	12.930	26.808	19.718	4.963	-126.969	-111.195	34.716
800	13.120	28.548	20.715	6.266	-126.950	-108.944	29.762
828	13.162	29.000	20.988	6.634	-126.953	-108.313	28.589
828	13.162	29.000	20.988	6.634	-127.133	-108.313	28.589
900	13.270	30.101	21.673	7.585	-127.147	-106.676	25.904
1000	13.440	31.509	22.588	8.921	-127.155	-104.401	22.816
1041	13.493	32.050	22.950	9.473	-127.155	-103.467	21.722
1041	13.493	32.050	22.950	9.473	-129.115	-103.467	21.722
1100	13.570	32.796	23.459	10.271	-129.077	-102.015	20.268
1200	13.700	33.982	24.286	11.635	-129.003	-99.557	18.132
1300	13.831	35.084	25.076	13.011	-128.922	-97.108	16.325
1400	13.960	36.113	25.827	14.401	-128.831	-94.662	14.777
1500	14.086	37.081	26.546	15.803	-128.730	-92.227	13.437
1600	14.210	37.994	27.233	17.218	-128.621	-89.795	12.265
1654.1	14.274	38.468	27.592	17.989	-128.559	-88.485	11.691
1654.1	14.274	38.468	27.592	17.989	-161.289	-88.485	11.691
1700	14.329	38.859	27.891	18.645	-161.078	-86.469	11.116
1800	14.450	39.681	28.523	20.084	-160.609	-82.092	9.967
1900	14.575	40.466	29.132	21.535	-160.133	-77.742	8.942
2000	14.700	41.217	29.717	22.999	-159.650	-73.420	8.023

*Data above 298 K estimated.

Phase changes: 828 K, α - β 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.

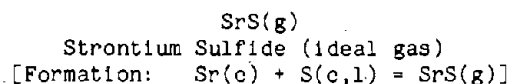
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $\text{Cp}^\circ = 12.021 + 1.416 \times 10^{-3}T - 0.714 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 12.021 \times 10^{-3}T + 0.708 \times 10^{-6}T^2 + 0.714 \times 10^{-2}T^{-1} - 3.886$

Reaction equations (kcal/mol):

298.15-828 K: $\Delta\text{Hr}^\circ = -128.360 + 3.255 \times 10^{-3}T - 1.984 \times 10^{-6}T^2 + 62.950T^{-1}$
 $\Delta\text{Gr}^\circ = -128.360 - 3.255 \times 10^{-3}T \ln T + 1.984 \times 10^{-6}T^2 + 31.475T^{-1} + 44.378 \times 10^{-3}T$
828-1041 K: $\Delta\text{Hr}^\circ = -126.597 - 1.151 \times 10^{-3}T + 0.548 \times 10^{-6}T^2 + 37.250T^{-1}$
 $\Delta\text{Gr}^\circ = -126.597 + 1.151 \times 10^{-3}T \ln T - 0.548 \times 10^{-6}T^2 + 18.625T^{-1} + 14.760 \times 10^{-3}T$
1041-1654.1 K: $\Delta\text{Hr}^\circ = -129.182 - 0.551 \times 10^{-3}T + 0.548 \times 10^{-6}T^2 + 37.250T^{-1}$
 $\Delta\text{Gr}^\circ = -129.182 + 0.551 \times 10^{-3}T \ln T - 0.548 \times 10^{-6}T^2 + 18.625T^{-1} + 21.411 \times 10^{-3}T$
1654.1-2000 K: $\Delta\text{Hr}^\circ = -158.059 - 2.424 \times 10^{-3}T + 1.523 \times 10^{-6}T^2 - 5623.450T^{-1}$
 $\Delta\text{Gr}^\circ = -158.059 + 2.424 \times 10^{-3}T \ln T - 1.523 \times 10^{-6}T^2 - 2811.725T^{-1} + 27.636 \times 10^{-3}T$

Source: Data from Chase (17) who estimated all above 298 K.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	8.479	58.078	58.078	0	25.860	14.555	-10.669
300	8.485	58.130	58.078	.016	25.854	14.486	-10.553
368.3	8.622	59.887	58.257	.601	25.609	11.922	-7.074
368.3	8.622	59.887	58.257	.601	25.513	11.922	-7.074
388.36	8.663	60.346	58.353	.774	25.433	11.184	-6.294
388.36	8.663	60.346	58.353	.774	25.020	11.184	-6.294
400	8.686	60.602	58.415	.875	24.954	10.770	-5.885
432.02	8.721	61.272	58.602	1.154	24.750	9.642	-4.878
500	8.794	62.553	59.053	1.750	24.193	7.311	-3.196
600	8.861	64.163	59.775	2.633	23.477	4.002	-1.458
700	8.906	65.532	60.502	3.521	22.774	.812	-.253
717.824	8.912	65.756	60.630	3.680	22.649	.255	-.077

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $\text{Cp}^\circ = 7.759 + 1.562 \times 10^{-3}T + 0.225 \times 10^{-5}T^{-2}$
 $\text{H}^\circ - \text{H}^\circ_{298} = 7.759 \times 10^{-3}T + 0.781 \times 10^{-6}T^2 - 0.225 \times 10^{-2}T^{-1} - 2.307$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta \text{Hf}^\circ = 27.868 - 5.009 \times 10^{-3}T - 0.034 \times 10^{-6}T^2 - 152.400T^{-1}$
 $\Delta \text{Gf}^\circ = 27.868 + 5.009 \times 10^{-3}T \ln T + 0.034 \times 10^{-6}T^2 - 76.200T^{-1} - 72.343 \times 10^{-3}T$
 368.3-388.36 K: $\Delta \text{Hf}^\circ = 26.753 - 2.746 \times 10^{-3}T - 1.780 \times 10^{-6}T^2 + 3.200T^{-1}$
 $\Delta \text{Gf}^\circ = 26.753 + 2.746 \times 10^{-3}T \ln T + 1.780 \times 10^{-6}T^2 + 1.600T^{-1} - 57.160 \times 10^{-3}T$
 388.36-432.02 K: $\Delta \text{Hf}^\circ = 10.594 + 41.994 \times 10^{-3}T - 45.062 \times 10^{-6}T^2 + 1905.400T^{-1}$
 $\Delta \text{Gf}^\circ = 10.594 - 41.994 \times 10^{-3}T \ln T + 45.062 \times 10^{-6}T^2 + 952.700T^{-1} + 228.069 \times 10^{-3}T$
 432.02-717.824 K: $\Delta \text{Hf}^\circ = 1.116 + 38.088 \times 10^{-3}T - 25.250 \times 10^{-6}T^2 + 5131.900T^{-1}$
 $\Delta \text{Gf}^\circ = 1.116 - 38.088 \times 10^{-3}T \ln T + 25.250 \times 10^{-6}T^2 + 2565.950T^{-1} + 226.221 \times 10^{-3}T$

SrS(g)
Strontium Sulfide (ideal gas)
[Reaction: $\text{Sr(c,l,g)} + 0.5\text{S}_2(\text{g}) = \text{SrS(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	8.479	58.078	58.078	0	10.505	5.041	-3.695
300	8.485	58.130	58.078	.016	10.502	5.008	-3.648
400	8.686	60.602	58.415	.875	10.303	3.205	-1.751
500	8.794	62.553	59.053	1.750	10.066	1.458	-.637
600	8.861	64.163	59.775	2.633	9.783	-.239	.087
700	8.906	65.532	60.502	3.521	9.449	-1.884	.588
800	8.942	66.724	61.207	4.414	9.059	-3.476	.950
828	8.953	67.032	61.398	4.665	8.937	-3.913	1.033
828	8.953	67.032	61.398	4.665	8.757	-3.913	1.033
900	8.981	67.779	61.879	5.310	8.437	-5.001	1.214
1000	9.037	68.728	62.517	6.211	7.995	-6.469	1.414
1041	9.073	69.092	62.769	6.582	7.814	-7.059	1.482
1041	9.073	69.092	62.769	6.582	5.854	-7.059	1.482
1100	9.126	69.593	63.122	7.118	5.631	-7.785	1.547
1200	9.267	70.393	63.695	8.038	5.260	-8.987	1.637
1300	9.474	71.143	64.240	8.974	4.901	-10.162	1.708
1400	9.758	71.855	64.759	9.935	4.564	-11.307	1.765
1500	10.124	72.540	65.255	10.928	4.255	-12.431	1.811
1600	10.567	73.207	65.731	11.962	3.983	-13.532	1.848
1654.1	10.843	73.563	65.981	12.541	3.853	-14.124	1.866
1654.1	10.843	73.563	65.981	12.541	-28.877	-14.124	1.866
1700	11.077	73.863	66.190	13.044	-28.819	-13.717	1.763
1800	11.637	74.511	66.634	14.179	-28.654	-12.831	1.558
1900	12.226	75.156	67.065	15.372	-28.436	-11.956	1.375
2000	12.821	75.799	67.487	16.625	-28.163	-11.098	1.213

Phase changes: 828 K, α - β 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.

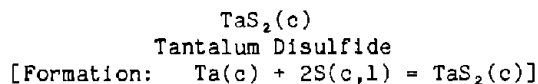
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 7.759 + 1.562 \times 10^{-3}T + 0.225 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 7.759 \times 10^{-3}T + 0.781 \times 10^{-6}T^2 - 0.225 \times 10^{-2}T^{-1} - 2.307$

Reaction equations (kcal/mol):

298.15-828 K: $\Delta H_r^\circ = 11.079 - 1.007 \times 10^{-3}T - 1.911 \times 10^{-6}T^2 - 30.950T^{-1}$
 $\Delta G_r^\circ = 11.079 + 1.007 \times 10^{-3}T \ln T + 1.911 \times 10^{-6}T^2 - 15.475T^{-1} - 26.380 \times 10^{-3}T$
828-1041 K: $\Delta H_r^\circ = 12.842 - 5.412 \times 10^{-3}T + 0.621 \times 10^{-6}T^2 - 56.650T^{-1}$
 $\Delta G_r^\circ = 12.842 + 5.412 \times 10^{-3}T \ln T - 0.621 \times 10^{-6}T^2 - 28.325T^{-1} - 55.998 \times 10^{-3}T$
1041-1654.1 K: $\Delta H_r^\circ = 10.257 - 4.813 \times 10^{-3}T + 0.621 \times 10^{-6}T^2 - 56.650T^{-1}$
 $\Delta G_r^\circ = 10.257 + 4.813 \times 10^{-3}T \ln T - 0.621 \times 10^{-6}T^2 - 28.325T^{-1} - 49.346 \times 10^{-3}T$
1654.1-2000 K: $\Delta H_r^\circ = -18.620 - 6.686 \times 10^{-3}T + 1.596 \times 10^{-6}T^2 - 5717.350T^{-1}$
 $\Delta G_r^\circ = -18.620 + 6.686 \times 10^{-3}T \ln T - 1.596 \times 10^{-6}T^2 - 2858.675T^{-1} - 43.122 \times 10^{-3}T$

Source: Data from Chase (17) who estimated some molecular constants.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	16.610	18.000	18.000	0	-84.600	-82.441	60.430
300	16.620	18.100	18.000	.030	-84.601	-82.426	60.047
368.3	17.002	21.549	18.350	1.178	-84.640	-81.930	48.617
368.3	17.002	21.549	18.350	1.178	-84.832	-81.930	48.617
388.36	17.115	22.454	18.539	1.520	-84.852	-81.770	46.016
388.36	17.115	22.454	18.539	1.520	-85.678	-81.770	46.016
400	17.180	22.960	18.660	1.720	-85.727	-81.653	44.612
432.02	17.343	24.289	19.029	2.273	-85.900	-81.321	41.138
500	17.690	26.850	19.910	3.470	-86.476	-80.542	35.205
600	18.170	30.120	21.353	5.260	-87.030	-79.304	28.886
700	18.650	32.960	22.817	7.100	-87.426	-77.987	24.348
717.824	18.734	33.430	23.075	7.433	-87.481	-77.745	23.670

*Entropy at 298 K estimated.

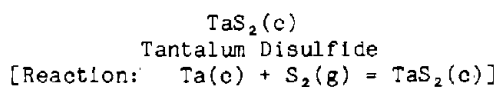
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1800 K: Cp° = 15.469 + 4.602x10⁻³T - 0.204x10⁻⁵T⁻²
H° - H°₂₉₈ = 15.469x10⁻³T + 2.301x10⁻⁶T² + 0.204x10⁻²T⁻¹ - 4.885

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -82.483 - 5.935x10⁻³T + 5.053x10⁻⁶T² - 237.600T⁻¹
ΔGf° = -82.483 + 5.935x10⁻³TlnT - 5.053x10⁻⁶T² - 118.800T⁻¹ - 30.832x10⁻³T
368.3-388.36 K: ΔHf° = -84.713 - 1.409x10⁻³T + 1.561x10⁻⁶T² + 73.600T⁻¹
ΔGf° = -84.713 + 1.409x10⁻³TlnT - 1.561x10⁻⁶T² + 36.800T⁻¹ - 0.466x10⁻³T
388.36-432.02 K: ΔHf° = -117.030 + 88.071x10⁻³T - 85.003x10⁻⁶T² + 3878.000T⁻¹
ΔGf° = -117.030 - 88.071x10⁻³TlnT + 85.003x10⁻⁶T² + 1939.000T⁻¹ + 569.991x10⁻³T
432.02-717.824 K: ΔHf° = -135.987 + 80.259x10⁻³T - 45.379x10⁻⁶T² + 10331.000T⁻¹
ΔGf° = -135.987 - 80.259x10⁻³TlnT + 45.379x10⁻⁶T² + 5165.500T⁻¹ + 566.296x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	16.610	18.000	18.000	0	-115.310	-101.468	74.377
300	16.620	18.100	18.000	.030	-115.305	-101.381	73.855
400	17.180	22.960	18.660	1.720	-115.029	-96.784	52.880
500	17.690	26.850	19.910	3.470	-114.731	-92.249	40.321
600	18.170	30.120	21.353	5.260	-114.419	-87.786	31.976
700	18.650	32.960	22.817	7.100	-114.076	-83.378	26.031
800	19.120	35.480	24.243	8.990	-113.699	-79.014	21.585
900	19.590	37.760	25.627	10.920	-113.297	-74.710	18.142
1000	20.050	39.850	26.940	12.910	-112.848	-70.440	15.394
1100	20.510	41.780	28.207	14.930	-112.383	-66.227	13.158
1200	20.980	43.580	29.405	17.010	-111.871	-62.041	11.299
1300	21.440	45.280	30.565	19.130	-111.333	-57.915	9.736
1400	21.900	46.890	31.676	21.300	-110.761	-53.830	8.403
1500	22.360	48.410	32.737	23.510	-110.165	-49.778	7.253
1600	22.820	49.870	33.764	25.770	-109.535	-45.775	6.252
1700	23.290	51.270	34.758	28.070	-108.882	-41.820	5.376
1800	23.750	52.610	35.704	30.430	-108.183	-37.879	4.599

*Entropy at 298 K estimated.

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

$$298.15-1800 \text{ K: } \begin{aligned} \text{Cp}^\circ &= 15.469 + 4.602 \times 10^{-3} T - 0.204 \times 10^{-5} T^2 \\ \text{H}^\circ - \text{H}_{298}^\circ &= 15.469 \times 10^{-3} T + 2.301 \times 10^{-6} T^2 + 0.204 \times 10^{-2} T^{-1} - 4.885 \end{aligned}$$

Reaction equations (kcal/mol):

$$298.15-1800 \text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= -116.060 + 2.070 \times 10^{-3} T + 1.299 \times 10^{-6} T^2 + 5.300 T^{-1} \\ \Delta \text{Gr}^\circ &= -116.060 - 2.070 \times 10^{-3} T \ln T - 1.299 \times 10^{-6} T^2 + 2.650 T^{-1} + 61.094 \times 10^{-3} T \end{aligned}$$

Sources: Enthalpy of formation and estimated entropy at 298 K from Mills (80). Other data based on Volovik (125).

TbS(g)
Terbium Monosulfide (ideal gas)
[Formation: $\text{Tb(c)} + \text{S(c,l)} = \text{TbS(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	8.200	63.820	63.820	0	37.700	26.180	-19.190
300	8.210	63.870	63.820	.015	37.692	26.108	-19.019
368.3	8.415	65.581	63.994	.585	37.409	23.499	-13.944
368.3	8.415	65.581	63.994	.585	37.313	23.499	-13.944
388.36	8.475	66.029	64.087	.754	37.227	22.749	-12.802
388.36	8.475	66.029	64.087	.754	36.814	22.749	-12.802
400	8.510	66.280	64.147	.853	36.745	22.329	-12.200
432.02	8.555	66.937	64.330	1.126	36.537	21.182	-10.715
500	8.650	68.190	64.766	1.712	35.987	18.811	-8.222
600	8.730	69.780	65.478	2.581	35.303	15.438	-5.623
700	8.780	71.130	66.193	3.456	34.645	12.179	-3.802
717.824	8.785	71.351	66.318	3.613	34.530	11.609	-3.535

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.

388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.

432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.

717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $C_p^\circ = 8.875 + 0.036 \times 10^{-3} T - 0.608 \times 10^{-5} T^2$
 $H^\circ - H_{298}^\circ = 8.875 \times 10^{-3} T + 0.018 \times 10^{-6} T^2 + 0.608 \times 10^{-2} T^{-1} - 2.852$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 38.713 - 3.583 \times 10^{-3} T - 0.379 \times 10^{-6} T^2 + 26.600 T^{-1}$
 $\Delta G_f^\circ = 38.713 + 3.583 \times 10^{-3} T \ln T + 0.379 \times 10^{-6} T^2 + 13.300 T^{-1} - 62.713 \times 10^{-3} T$
368.3-388.36 K: $\Delta H_f^\circ = 37.598 - 1.320 \times 10^{-3} T - 2.125 \times 10^{-6} T^2 + 182.200 T^{-1}$
 $\Delta G_f^\circ = 37.598 + 1.320 \times 10^{-3} T \ln T + 2.125 \times 10^{-6} T^2 + 91.100 T^{-1} - 47.530 \times 10^{-3} T$
388.36-432.02 K: $\Delta H_f^\circ = 21.439 + 43.420 \times 10^{-3} T - 45.407 \times 10^{-6} T^2 + 2084.400 T^{-1}$
 $\Delta G_f^\circ = 21.439 - 43.420 \times 10^{-3} T \ln T + 45.407 \times 10^{-6} T^2 + 1042.200 T^{-1} + 237.698 \times 10^{-3} T$
432.02-717.824 K: $\Delta H_f^\circ = 11.961 + 39.514 \times 10^{-3} T - 25.595 \times 10^{-6} T^2 + 5310.900 T^{-1}$
 $\Delta G_f^\circ = 11.961 - 39.514 \times 10^{-3} T \ln T + 25.595 \times 10^{-6} T^2 + 2655.450 T^{-1} + 235.851 \times 10^{-3} T$

TbS(g)
Terbium Monosulfide (ideal gas)
[Reaction: $\text{Tb(c,l)} + 0.5\text{S}_2(\text{g}) = \text{TbS(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15*	8.200	63.820	63.820	0	22.345	16.666	-12.216
300	8.210	63.870	63.820	.015	22.340	16.630	-12.115
400	8.510	66.280	64.147	.853	22.094	14.763	-8.066
500	8.650	68.190	64.766	1.712	21.860	12.957	-5.664
600	8.730	69.780	65.478	2.581	21.609	11.197	-4.079
700	8.780	71.130	66.193	3.456	21.320	9.484	-2.961
800	8.810	72.300	66.881	4.335	20.997	7.823	-2.137
900	8.830	73.340	67.543	5.217	20.638	6.193	-1.504
1000	8.850	74.270	68.168	6.102	20.239	4.608	-1.007
1100	8.860	75.120	68.768	6.987	19.802	3.065	-.609
1200	8.880	75.890	69.328	7.874	19.324	1.561	-.284
1300	8.880	76.600	69.860	8.762	18.798	.105	-.018
1400	8.890	77.260	70.366	9.651	18.222	-1.307	.204
1500	8.900	77.870	70.843	10.541	17.592	-2.674	.390
1560	8.906	78.224	71.125	11.076	17.183	-3.491	.489
1560	8.906	78.224	71.125	11.076	15.983	-3.491	.489
1600	8.910	78.450	71.305	11.432	15.888	-3.984	.544
1630	8.910	78.616	71.438	11.699	15.815	-4.364	.585
1630	8.910	78.616	71.438	11.699	13.235	-4.364	.585
1700	8.910	78.990	71.741	12.323	12.750	-5.110	.657
1800	8.920	79.500	72.159	13.214	12.059	-6.149	.747
1900	8.930	79.980	72.555	14.107	11.365	-7.138	.821
2000	8.930	80.440	72.940	15.000	10.668	-8.098	.885

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 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:

298.15-2000 K: $\text{Cp}^\circ = 8.875 + 0.036 \times 10^{-3}T - 0.608 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 8.875 \times 10^{-3}T + 0.018 \times 10^{-6}T^2 + 0.608 \times 10^{-2}T^{-1} - 2.852$

Reaction equations (kcal/mol):

298.15-1560 K: $\Delta\text{Hr}^\circ = 21.924 + 0.420 \times 10^{-3}T - 2.256 \times 10^{-6}T^2 + 148.050T^{-1}$
 $\Delta\text{Gr}^\circ = 21.924 - 0.420 \times 10^{-3}T \ln T + 2.256 \times 10^{-6}T^2 + 74.025T^{-1} - 16.750 \times 10^{-3}T$
1560-1630 K: $\Delta\text{Hr}^\circ = 19.334 - 1.937 \times 10^{-3}T - 0.142 \times 10^{-6}T^2 + 26.650T^{-1}$
 $\Delta\text{Gr}^\circ = 19.334 + 1.937 \times 10^{-3}T \ln T + 0.142 \times 10^{-6}T^2 + 13.325T^{-1} - 29.097 \times 10^{-3}T$
1630-2000 K: $\Delta\text{Hr}^\circ = 24.038 - 6.406 \times 10^{-3}T - 0.142 \times 10^{-6}T^2 + 26.650T^{-1}$
 $\Delta\text{Gr}^\circ = 24.038 + 6.406 \times 10^{-3}T \ln T + 0.142 \times 10^{-6}T^2 + 13.325T^{-1} - 65.037 \times 10^{-3}T$

Source: Data from Mills (80) who estimated all except enthalpy of formation at 298 K.

ThS(c)
Thorium Monosulfide
[Formation: Th(c) + S(c,l) = ThS(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	11.410	16.680	16.680	0	-95.500	-94.385	69.185
300*	11.420	16.751	16.681	.021	-95.501	-94.378	68.753
368.3	11.816	19.138	16.921	.817	-95.541	-94.118	55.849
368.3	11.816	19.138	16.921	.817	-95.637	-94.118	55.849
388.36	11.932	19.768	17.052	1.055	-95.653	-94.034	52.917
388.36	11.932	19.768	17.052	1.055	-96.066	-94.034	52.917
400	12.000	20.121	17.136	1.194	-96.093	-93.973	51.344
432.02	12.106	21.049	17.392	1.580	-96.188	-93.800	47.451
500	12.330	22.836	18.014	2.411	-96.500	-93.398	40.824
600	12.570	25.106	19.011	3.657	-96.818	-92.745	33.782
700	12.760	27.059	20.025	4.924	-97.078	-92.046	28.738
717.824	12.789	27.380	20.203	5.152	-97.119	-91.917	27.985

*Data above 298 K estimated.

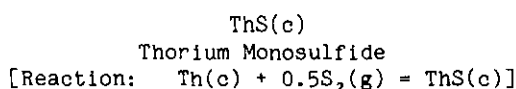
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 12.054 + 1.260x10⁻³T - 0.906x10⁻⁵T⁻²
H°- H₂₉₈° = 12.054x10⁻³T + 0.630x10⁻⁶T² + 0.906x10⁻²T⁻¹ - 3.954

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -94.731 - 2.178x10⁻³T + 1.400x10⁻⁶T² - 72.900T⁻¹
ΔGf° = -94.731 + 2.178x10⁻³T ln T - 1.400x10⁻⁶T² - 36.450T⁻¹ - 10.422x10⁻³T
368.3-388.36 K: ΔHf° = -95.846 + 0.085x10⁻³T - 0.346x10⁻⁶T² + 82.700T⁻¹
ΔGf° = -95.846 - 0.085x10⁻³T ln T + 0.346x10⁻⁶T² + 41.350T⁻¹ + 4.761x10⁻³T
388.36-432.02 K: ΔHf° = -112.004 + 44.825x10⁻³T - 43.628x10⁻⁶T² + 1984.900T⁻¹
ΔGf° = -112.004 - 44.825x10⁻³T ln T + 43.628x10⁻⁶T² + 992.450T⁻¹ + 289.990x10⁻³T
432.02-717.824 K: ΔHf° = -121.483 + 40.919x10⁻³T - 23.816x10⁻⁶T² + 5211.400T⁻¹
ΔGf° = -121.483 - 40.919x10⁻³T ln T + 23.816x10⁻⁶T² + 2605.700T⁻¹ + 288.142x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	11.410	16.680	16.680	0	-110.855	-103.898	76.159
300*	11.420	16.751	16.681	.021	-110.853	-103.855	75.657
400	12.000	20.121	17.136	1.194	-110.744	-101.539	55.477
500	12.330	22.836	18.014	2.411	-110.627	-99.251	43.382
600	12.570	25.106	19.011	3.657	-110.513	-96.986	35.327
700	12.760	27.059	20.025	4.924	-110.403	-94.741	29.579
800	12.920	28.773	21.013	6.208	-110.300	-92.509	25.272
900	13.070	30.303	21.962	7.507	-110.209	-90.292	21.926
1000	13.220	31.688	22.866	8.822	-110.122	-88.083	19.250
1100	13.350	32.954	23.727	10.150	-110.046	-85.883	17.063
1200	13.490	34.122	24.545	11.492	-109.979	-83.691	15.242
1300	13.630	35.207	25.324	12.848	-109.919	-81.501	13.701
1400	13.760	36.222	26.066	14.218	-109.868	-79.316	12.382
1500	13.900	37.176	26.775	15.601	-109.828	-77.137	11.239
1600	14.030	38.077	27.454	16.997	-109.795	-74.958	10.239
1633	14.076	38.364	27.671	17.461	-109.787	-74.240	9.936
1633	14.076	38.364	27.671	17.461	-110.647	-74.240	9.936
1700	14.170	38.932	28.104	18.407	-110.586	-72.748	9.352
1800	14.310	39.746	28.729	19.831	-110.509	-70.525	8.563
1900	14.460	40.524	29.329	21.270	-110.450	-68.305	7.857
2000	14.600	41.269	29.908	22.723	-110.409	-66.089	7.222

*Data above 298 K estimated.

Phase change: 1633 K, α - β transition point of Th; ΔH° = 0.860 kcal/mol.

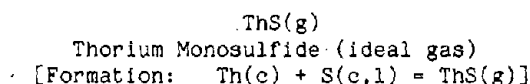
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $\text{Cp}^\circ = 12.054 + 1.260 \times 10^{-3}T - 0.906 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 12.054 \times 10^{-3}T + 0.630 \times 10^{-6}T^2 + 0.906 \times 10^{-2}T^{-1} - 3.954$

Reaction equations (kcal/mol):

298.15-1633 K: $\Delta\text{Hr}^\circ = -111.519 + 1.825 \times 10^{-3}T - 0.477 \times 10^{-6}T^2 + 48.550T^{-1}$
 $\Delta\text{Gr}^\circ = -111.519 - 1.825 \times 10^{-3}T \ln T + 0.477 \times 10^{-6}T^2 + 24.275T^{-1} + 35.541 \times 10^{-3}T$
 1633-2000 K: $\Delta\text{Hr}^\circ = -114.768 + 4.073 \times 10^{-3}T - 0.948 \times 10^{-6}T^2 + 2.950T^{-1}$
 $\Delta\text{Gr}^\circ = -114.768 - 4.073 \times 10^{-3}T \ln T + 0.948 \times 10^{-6}T^2 + 1.475T^{-1} + 53.409 \times 10^{-3}T$

Source: Data from Gronvold (47) who estimated all above 298 K.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	8.250	60.310	60.310	0	72.000	60.107	-44.059
300	8.256	60.361	60.311	.015	71.993	60.033	-43.734
368.3	8.433	62.074	60.482	.586	71.729	57.338	-34.024
368.3	8.433	62.074	60.482	.586	71.633	57.338	-34.024
388.36	8.485	62.523	60.576	.756	71.549	56.563	-31.830
388.36	8.485	62.523	60.576	.756	71.136	56.563	-31.830
400	8.515	62.774	60.636	.855	71.068	56.127	-30.666
432.02	8.563	63.432	60.820	1.128	70.861	54.938	-27.792
500	8.664	64.691	61.263	1.714	70.303	52.477	-22.938
600	8.788	66.281	61.971	2.586	69.611	48.979	-17.840
700	8.947	67.647	62.687	3.472	68.970	45.591	-14.234
717.824	8.988	67.872	62.813	3.632	68.861	44.997	-13.700

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: $C_p^\circ = 6.918 + 3.026 \times 10^{-3}T + 0.382 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 6.918 \times 10^{-3}T + 1.513 \times 10^{-6}T^2 - 0.382 \times 10^{-2}T^{-1} - 2.069$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 74.654 - 7.314 \times 10^{-3}T + 2.283 \times 10^{-6}T^2 - 201.700T^{-1}$
 $\Delta G_f^\circ = 74.654 + 7.314 \times 10^{-3}T \ln T - 2.283 \times 10^{-6}T^2 - 100.850T^{-1} - 88.648 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = 73.539 - 5.051 \times 10^{-3}T + 0.537 \times 10^{-6}T^2 - 46.100T^{-1}$
 $\Delta G_f^\circ = 73.539 + 5.051 \times 10^{-3}T \ln T - 0.537 \times 10^{-6}T^2 - 23.050T^{-1} - 73.465 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = 57.381 + 39.689 \times 10^{-3}T - 42.745 \times 10^{-6}T^2 + 1856.100T^{-1}$
 $\Delta G_f^\circ = 57.381 - 39.689 \times 10^{-3}T \ln T + 42.745 \times 10^{-6}T^2 + 928.050T^{-1} + 211.763 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = 47.902 + 35.783 \times 10^{-3}T - 22.933 \times 10^{-6}T^2 + 5082.600T^{-1}$
 $\Delta G_f^\circ = 47.902 - 35.783 \times 10^{-3}T \ln T + 22.933 \times 10^{-6}T^2 + 2541.300T^{-1} + 209.915 \times 10^{-3}T$

ThS(g)
Thorium Monosulfide (ideal gas)
[Reaction: Th(c) + 0.5S₂(g) = ThS(g)]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	8.250	60.310	60.310	0	56.645	50.593	-37.086
300	8.256	60.361	60.311	.015	56.641	50.556	-36.830
400	8.515	62.774	60.636	.855	56.417	48.561	-26.532
500	8.664	64.691	61.263	1.714	56.175	46.624	-20.379
600	8.788	66.281	61.971	2.586	55.917	44.738	-16.296
700	8.947	67.647	62.687	3.472	55.645	42.896	-13.392
800	9.178	68.855	63.383	4.378	55.369	41.095	-11.227
900	9.490	69.954	64.053	5.311	55.095	39.326	-9.549
1000	9.870	70.973	64.695	6.278	54.834	37.588	-8.215
1100	10.288	71.933	65.309	7.286	54.591	35.876	-7.128
1200	10.709	72.847	65.900	8.336	54.365	34.183	-6.226
1300	11.103	73.720	66.468	9.427	54.160	32.511	-5.466
1400	11.444	74.556	67.017	10.555	53.969	30.853	-4.816
1500	11.719	75.355	67.546	11.714	53.785	29.207	-4.255
1600	11.922	76.118	68.057	12.897	53.605	27.576	-3.767
1633	11.966	76.362	68.223	13.291	53.544	27.040	-3.619
1633	11.966	76.362	68.223	13.291	52.684	27.040	-3.619
1700	12.054	76.845	68.553	14.096	52.604	25.989	-3.341
1800	12.121	77.536	69.033	15.305	52.465	24.427	-2.966
1900	12.132	78.192	69.498	16.518	52.298	22.874	-2.631
2000	12.098	78.814	69.949	17.730	52.099	21.328	-2.331

*Data except enthalpy of formation at 298 K estimated.

Phase change: 1633 K, α - β transition point of Th; ΔH° = 0.860 kcal/mol.

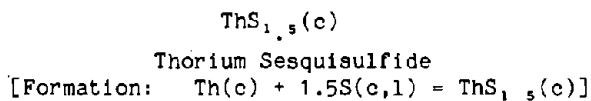
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

$$298.15-2000 \text{ K: } \begin{aligned} \text{Cp}^\circ &= 6.918 + 3.026 \times 10^{-3}T + 0.382 \times 10^{-5}T^2 \\ \text{H}^\circ - \text{H}_{298}^\circ &= 6.918 \times 10^{-3}T + 1.513 \times 10^{-6}T^2 - 0.382 \times 10^{-3}T^{-1} - 2.069 \end{aligned}$$

Reaction equations (kcal/mol):

$$\begin{aligned} 298.15-1633 \text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= 57.865 - 3.312 \times 10^{-3}T + 0.406 \times 10^{-6}T^2 - 80.250T^{-1} \\ \Delta \text{Gr}^\circ &= 57.865 + 3.312 \times 10^{-3}T \ln T - 0.406 \times 10^{-6}T^2 - 40.125T^{-1} - 42.685 \times 10^{-3}T \end{aligned} \\ 1633-2000 \text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= 54.617 - 1.063 \times 10^{-3}T - 0.065 \times 10^{-6}T^2 - 125.850T^{-1} \\ \Delta \text{Gr}^\circ &= 54.617 + 1.063 \times 10^{-3}T \ln T + 0.065 \times 10^{-6}T^2 - 62.925T^{-1} - 24.818 \times 10^{-3}T \end{aligned} \end{aligned}$$

Source: Data from Gronvold (47) who estimated all except enthalpy of formation at 298 K.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15*	14.606	21.500	21.500	0	-129.500	-128.680	94.324
300	14.615	21.590	21.500	.027	-129.500	-128.674	93.738
368.3	14.887	24.618	21.807	1.035	-129.520	-128.486	76.243
368.3	14.887	24.618	21.807	1.035	-129.664	-128.486	76.243
388.36	14.967	25.409	21.973	1.335	-129.677	-128.420	72.268
388.36	14.967	25.409	21.973	1.335	-130.297	-128.420	72.268
400	15.013	25.852	22.080	1.509	-130.333	-128.364	70.134
432.02	15.105	27.012	22.403	1.991	-130.463	-128.202	64.854
500	15.300	29.234	23.184	3.025	-130.910	-127.807	55.864
600	15.530	32.044	24.432	4.567	-131.360	-127.141	46.311
700	15.743	34.454	25.695	6.131	-131.723	-126.409	39.466
717.824	15.779	34.850	25.918	6.412	-131.779	-126.272	38.445

*Data except enthalpy of formation at 298 K estimated.

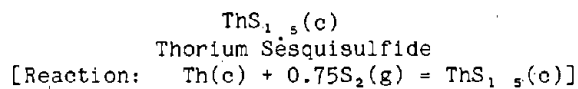
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 14.576 + 1.798x10⁻³T - 0.450x10⁻⁵T²
 H° - H₂₉₈° = 14.576x10⁻³T + 0.899x10⁻⁶T² + 0.450x10⁻²T⁻¹ - 4.577

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -127.950 - 3.743x10⁻³T + 2.528x10⁻⁶T² - 196.300T⁻¹
 ΔGf° = -127.950 + 3.743x10⁻³TlnT - 2.528x10⁻⁶T² - 98.150T⁻¹ - 21.915x10⁻³T
 368.3-388.36 K: ΔHf° = -129.623 - 0.348x10⁻³T - 0.091x10⁻⁶T² + 37.100T⁻¹
 ΔGf° = -129.623 + 0.348x10⁻³TlnT + 0.091x10⁻⁶T² + 18.550T⁻¹ + 0.860x10⁻³T
 388.36-432.02 K: ΔHf° = -153.860 + 66.761x10⁻³T - 65.015x10⁻⁶T² + 2890.400T⁻¹
 ΔGf° = -153.860 - 66.761x10⁻³TlnT + 65.015x10⁻⁶T² + 1445.200T⁻¹ + 428.702x10⁻³T
 432.02-717.824 K: ΔHf° = -168.078 + 60.903x10⁻³T - 35.297x10⁻⁶T² + 7730.150T⁻¹
 ΔGf° = -168.078 - 60.903x10⁻³TlnT + 35.297x10⁻⁶T² + 3865.075T⁻¹ + 425.931x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15*	14.606	21.500	21.500	0	-152.533	-142.950	104.784
300	14.615	21.590	21.500	.027	-152.528	-142.890	104.094
400	15.013	25.852	22.080	1.509	-152.309	-139.712	76.334
500	15.300	29.234	23.184	3.025	-152.101	-136.587	59.701
600	15.530	32.044	24.432	4.567	-151.902	-133.503	48.628
700	15.743	34.454	25.695	6.131	-151.711	-130.451	40.728
800	15.944	36.570	26.926	7.715	-151.526	-127.426	34.811
900	16.140	38.459	28.103	9.320	-151.348	-124.426	30.214
1000	16.330	40.169	29.226	10.943	-151.175	-121.443	26.541
1100	16.518	41.734	30.293	12.585	-151.008	-118.477	23.539
1200	16.703	43.180	31.308	14.247	-150.847	-115.528	21.040
1300	16.888	44.524	32.273	15.926	-150.691	-112.590	18.928
1400	17.072	45.782	33.193	17.624	-150.542	-109.664	17.119
1500	17.255	46.966	34.073	19.340	-150.399	-106.752	15.554
1600	17.437	48.086	34.914	21.075	-150.261	-103.846	14.185
1633	17.497	48.443	35.184	21.651	-150.217	-102.890	13.770
1633	17.497	48.443	35.184	21.651	-151.077	-102.890	13.770
1700	17.619	49.148	35.720	22.828	-150.943	-100.914	12.973
1800	17.801	50.161	36.495	24.599	-150.756	-97.978	11.896
1900	17.982	51.128	37.240	26.388	-150.584	-95.050	10.933
2000	18.163	52.055	37.958	28.195	-150.428	-92.133	10.068

*Data except enthalpy of formation at 298 K estimated.

Phase change: 1633 K, α - β transition point of Th; ΔH° = 0.860 kcal/mol.

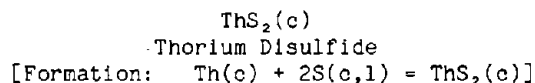
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 14.576 + 1.798 \times 10^{-3}T - 0.450 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 14.576 \times 10^{-3}T + 0.899 \times 10^{-6}T^2 + 0.450 \times 10^{-2}T^{-1} - 4.577$

Reaction equations (kcal/mol):

298.15-1633 K: $\Delta H_r^\circ = -153.134 + 2.261 \times 10^{-3}T - 0.288 \times 10^{-6}T^2 - 14.125T^{-1}$
 $\Delta G_r^\circ = -153.134 - 2.261 \times 10^{-3}T \ln T + 0.288 \times 10^{-6}T^2 - 7.063T^{-1} + 47.030 \times 10^{-3}T$
1633-2000 K: $\Delta H_r^\circ = -156.382 + 4.510 \times 10^{-3}T - 0.759 \times 10^{-6}T^2 - 59.725T^{-1}$
 $\Delta G_r^\circ = -156.382 - 4.510 \times 10^{-3}T \ln T + 0.759 \times 10^{-6}T^2 - 29.862T^{-1} + 64.897 \times 10^{-3}T$

Source: Data from Gronvold (47) who estimated all except enthalpy of formation at 298 K.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	16.800	23.000	23.000	0	-150	-148.485	108.841
300*	16.840	23.104	23.001	.031	-150.001	-148.475	108.163
368.3	17.277	26.607	23.354	1.198	-150.054	-148.123	87.895
368.3	17.277	26.607	23.354	1.198	-150.246	-148.123	87.895
388.36	17.406	27.527	23.546	1.546	-150.270	-148.006	83.289
388.36	17.406	27.527	23.546	1.546	-151.096	-148.006	83.289
400	17.480	28.042	23.670	1.749	-151.148	-147.913	80.815
432.02	17.611	29.393	24.044	2.311	-151.330	-147.648	74.691
500	17.890	31.989	24.951	3.519	-151.939	-147.015	64.259
600	18.160	35.275	26.405	5.322	-152.557	-145.968	53.168
700	18.390	38.093	27.879	7.150	-153.056	-144.830	45.217
717.824	18.420	38.556	28.138	7.478	-153.134	-144.619	44.031

*Data above 298 K estimated.

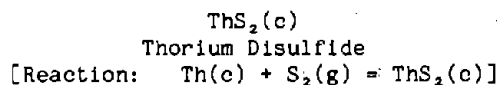
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: $C_p^\circ = 17.417 + 1.614 \times 10^{-3}T - 0.976 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 17.417 \times 10^{-3}T + 0.807 \times 10^{-6}T^2 + 0.976 \times 10^{-2}T^{-1} - 5.592$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -148.062 - 4.989 \times 10^{-3}T + 3.294 \times 10^{-6}T^2 - 221.500T^{-1}$
 $\Delta G_f^\circ = -148.062 + 4.989 \times 10^{-3}T \ln T - 3.294 \times 10^{-6}T^2 - 110.750T^{-1} - 27.614 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = -150.293 - 0.463 \times 10^{-3}T - 0.198 \times 10^{-6}T^2 + 89.700T^{-1}$
 $\Delta G_f^\circ = -150.293 + 0.463 \times 10^{-3}T \ln T + 0.198 \times 10^{-6}T^2 + 44.850T^{-1} + 2.752 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = -182.609 + 89.017 \times 10^{-3}T - 86.762 \times 10^{-6}T^2 + 3894.100T^{-1}$
 $\Delta G_f^\circ = -182.609 - 89.017 \times 10^{-3}T \ln T + 86.762 \times 10^{-6}T^2 + 1947.050T^{-1} + 573.209 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = -201.567 + 81.205 \times 10^{-3}T - 47.138 \times 10^{-6}T^2 + 10347.100T^{-1}$
 $\Delta G_f^\circ = -201.567 - 81.205 \times 10^{-3}T \ln T + 47.138 \times 10^{-6}T^2 + 5173.550T^{-1} + 569.514 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	16.800	23.000	23.000	0	-180.710	-167.512	122.788
300*	16.840	23.104	23.001	.031	-180.705	-167.430	121.971
400	17.480	28.042	23.670	1.749	-180.450	-163.044	89.082
500	17.890	31.989	24.951	3.519	-180.194	-158.721	69.376
600	18.160	35.275	26.405	5.322	-179.946	-154.450	56.258
700	18.390	38.093	27.879	7.150	-179.706	-150.221	46.900
800	18.560	40.559	29.313	8.997	-179.476	-146.022	39.891
900	18.790	42.759	30.687	10.865	-179.255	-141.856	34.447
1000	18.900	44.744	31.995	12.749	-179.043	-137.712	30.097
1100	19.050	46.553	33.238	14.647	-178.844	-133.588	26.541
1200	19.210	48.217	34.417	16.560	-178.657	-129.482	23.582
1300	19.370	49.761	35.539	18.489	-178.479	-125.391	21.080
1400	19.530	51.202	36.606	20.434	-178.312	-121.312	18.937
1500	19.690	52.555	37.625	22.395	-178.155	-117.249	17.083
1600	19.860	53.831	38.599	24.372	-178.007	-113.193	15.461
1633	19.916	54.237	38.910	25.028	-177.961	-111.857	14.970
1633	19.916	54.237	38.910	25.028	-178.821	-111.857	14.970
1700	20.030	55.040	39.530	26.367	-178.682	-109.111	14.027
1800	20.200	56.185	40.424	28.370	-178.499	-105.025	12.752
1900	21.380	57.318	41.284	30.465	-178.259	-100.950	11.612
2000	20.570	58.403	42.114	32.579	-178.035	-96.889	10.587

*Data above 298 K estimated.

Phase change: 1633 K, α - β transition point of Th; ΔH° = 0.860 kcal/mol.

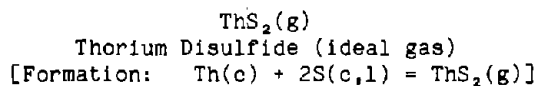
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $C_p^\circ = 17.417 + 1.614 \times 10^{-3}T - 0.976 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 17.417 \times 10^{-3}T + 0.807 \times 10^{-6}T^2 + 0.976 \times 10^{-2}T^{-1} - 5.592$

Reaction equations (kcal/mol):

298.15-1633 K: $\Delta H_r^\circ = -181.640 + 3.016 \times 10^{-3}T - 0.460 \times 10^{-6}T^2 + 21.400T^{-1}$
 $\Delta G_r^\circ = -181.640 - 3.016 \times 10^{-3}T \ln T + 0.460 \times 10^{-6}T^2 + 10.700T^{-1} + 64.312 \times 10^{-3}T$
1633-2000 K: $\Delta H_r^\circ = -184.889 + 5.265 \times 10^{-3}T - 0.931 \times 10^{-6}T^2 - 24.200T^{-1}$
 $\Delta G_r^\circ = -184.889 - 5.265 \times 10^{-3}T \ln T + 0.931 \times 10^{-6}T^2 - 12.100T^{-1} + 82.179 \times 10^{-3}T$

Source: Data from Gronvold (47) who estimated all above 298 K.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15*	12.685	72.630	72.630	0	18.000	4.718	-3.458
300	12.698	72.709	72.632	.023	17.991	4.635	-3.377
368.3	13.026	75.351	72.898	.904	17.652	1.630	-.967
368.3	13.026	75.351	72.898	.904	17.460	1.630	-.967
388.36	13.122	76.045	73.042	1.166	17.349	.772	-.434
388.36	13.122	76.045	73.042	1.166	16.523	.772	-.434
400	13.178	76.433	73.135	1.319	16.422	.301	-.164
432.02	13.257	77.451	73.418	1.742	16.102	-.979	.495
500	13.426	79.402	74.102	2.650	15.192	-3.590	1.569
600	13.567	81.863	75.196	4.000	14.121	-7.243	2.638
700	13.655	83.961	76.301	5.362	13.156	-10.726	3.349
717.824	13.666	84.304	76.495	5.605	12.994	-11.331	3.450

*Data estimated.

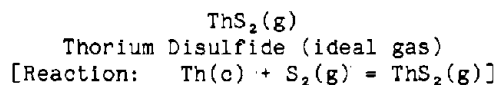
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 13.811 + 0.058x10⁻³T - 1.017x10⁻⁵T⁻²
 H° - H₂₉₈° = 13.811x10⁻³T + 0.029x10⁻⁶T² + 1.017x10⁻²T⁻¹ - 4.461

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 21.068 - 8.595x10⁻³T + 2.516x10⁻⁶T² - 217.400T⁻¹
 ΔGf° = 21.068 + 8.595x10⁻³T lnT - 2.516x10⁻⁶T² - 108.700T⁻¹ - 101.836x10⁻³T
 368.3-388.36 K: ΔHf° = 18.838 - 4.069x10⁻³T - 0.976x10⁻⁶T² + 93.800T⁻¹
 ΔGf° = 18.838 + 4.069x10⁻³T lnT + 0.976x10⁻⁶T² + 46.900T⁻¹ - 71.470x10⁻³T
 388.36-432.02 K: ΔHf° = -13.479 + 85.411x10⁻³T - 87.540x10⁻⁶T² + 3898.200T⁻¹
 ΔGf° = -13.479 - 85.411x10⁻³T lnT + 87.540x10⁻⁶T² + 1949.100T⁻¹ + 498.986x10⁻³T
 432.02-717.824 K: ΔHf° = -32.436 + 77.599x10⁻³T - 47.916x10⁻⁶T² + 10351.200T⁻¹
 ΔGf° = -32.436 - 77.599x10⁻³T lnT + 47.916x10⁻⁶T² + 5175.600T⁻¹ + 495.291x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	12.685	72.630	72.630	0	-12.710	-14.309	10.489
300	12.698	72.709	72.632	.023	-12.713	-14.319	10.431
400	13.178	76.433	73.135	1.319	-12.880	-14.830	8.103
500	13.426	79.402	74.102	2.650	-13.063	-15.297	6.686
600	13.567	81.863	75.196	4.000	-13.268	-15.725	5.728
700	13.655	83.961	76.301	5.362	-13.494	-16.116	5.032
800	13.714	85.789	77.377	6.730	-13.743	-16.473	4.500
900	13.754	87.407	78.403	8.104	-14.016	-16.801	4.080
1000	13.783	88.857	79.376	9.481	-14.311	-17.093	3.736
1100	13.805	90.172	80.299	10.860	-14.631	-17.356	3.448
1200	13.822	91.374	81.172	12.242	-14.975	-17.589	3.203
1300	13.835	92.481	82.001	13.624	-15.344	-17.792	2.991
1400	13.845	93.506	82.786	15.008	-15.738	-17.964	2.804
1500	13.853	94.462	83.533	16.393	-16.157	-18.111	2.639
1600	13.860	95.356	84.244	17.779	-16.600	-18.226	2.489
1633	13.862	95.639	84.472	18.236	-16.752	-18.257	2.443
1633	13.862	95.639	84.472	18.236	-17.612	-18.257	2.443
1700	13.866	96.197	84.923	19.165	-17.884	-18.280	2.350
1800	13.871	96.989	85.571	20.552	-18.317	-18.290	2.221
1900	13.875	97.739	86.192	21.940	-18.784	-18.275	2.102
2000	13.878	98.451	86.787	23.327	-19.287	-18.237	1.993

*Data 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: $C_p^\circ = 13.811 + 0.058 \times 10^{-3}T - 1.017 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 13.811 \times 10^{-3}T + 0.029 \times 10^{-6}T^2 + 1.017 \times 10^2 T^{-1} - 4.461$

Reaction equations (kcal/mol):

298.15-1633 K: $\Delta H_r^\circ = -12.510 - 0.590 \times 10^{-3}T - 1.238 \times 10^{-6}T^2 + 25.500T^{-1}$
 $\Delta G_r^\circ = -12.510 + 0.590 \times 10^{-3}T \ln T + 1.238 \times 10^{-6}T^2 + 12.750T^{-1} - 9.910 \times 10^{-3}T$
 1633-2000 K: $\Delta H_r^\circ = -15.758 + 1.659 \times 10^{-3}T - 1.709 \times 10^{-6}T^2 - 20.100T^{-1}$
 $\Delta G_r^\circ = -15.758 - 1.659 \times 10^{-3}T \ln T + 1.709 \times 10^{-6}T^2 - 10.050T^{-1} + 7.957 \times 10^{-3}T$

Source: Data are those estimated by Gronvold (47).

TiS(c)
Titanium Monosulfide
[Formation: $\text{Ti(c)} + \text{S(c,l)} = \text{TiS(c)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	11.490	13.500	13.500	0	-66.700	-66.258	48.568
300	11.500	13.570	13.500	.021	-66.700	-66.254	48.266
368.3	11.616	15.939	13.737	.811	-66.712	-66.152	39.254
368.3	11.616	15.939	13.737	.811	-66.808	-66.152	39.254
388.36	11.650	16.556	13.867	1.044	-66.818	-66.115	37.206
388.36	11.650	16.556	13.867	1.044	-67.231	-66.115	37.206
400	11.670	16.900	13.950	1.180	-67.257	-66.081	36.105
432.02	11.728	17.801	14.202	1.555	-67.349	-65.984	33.380
500	11.850	19.530	14.818	2.356	-67.661	-65.747	28.738
600	12.030	21.700	15.783	3.550	-67.988	-65.329	23.796
700	12.200	23.570	16.769	4.761	-68.266	-64.860	20.250
717.824	12.232	23.877	16.941	4.979	-68.311	-64.772	19.720

*Data except enthalpy of formation at 298 K estimated.

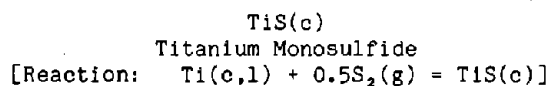
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: $C_p^\circ = 10.970 + 1.760 \times 10^{-3}T$
 $H^\circ - H_{298}^\circ = 10.970 \times 10^{-3}T + 0.880 \times 10^{-6}T^2 - 3.349$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -65.460 - 2.681 \times 10^{-3}T + 1.474 \times 10^{-6}T^2 - 170.400T^{-1}$
 $\Delta G_f^\circ = -65.460 + 2.681 \times 10^{-3}T \ln T - 1.474 \times 10^{-6}T^2 - 85.200T^{-1} - 16.555 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = -66.575 - 0.418 \times 10^{-3}T - 0.272 \times 10^{-6}T^2 - 14.800T^{-1}$
 $\Delta G_f^\circ = -66.575 + 0.418 \times 10^{-3}T \ln T + 0.272 \times 10^{-6}T^2 - 7.400T^{-1} - 1.372 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = -82.734 + 44.322 \times 10^{-3}T - 43.554 \times 10^{-6}T^2 + 1887.400T^{-1}$
 $\Delta G_f^\circ = -82.734 - 44.322 \times 10^{-3}T \ln T + 43.554 \times 10^{-6}T^2 + 943.700T^{-1} + 283.857 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = -92.212 + 40.416 \times 10^{-3}T - 23.742 \times 10^{-6}T^2 + 5113.900T^{-1}$
 $\Delta G_f^\circ = -92.212 - 40.416 \times 10^{-3}T \ln T + 23.742 \times 10^{-6}T^2 + 2556.950T^{-1} + 282.009 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	11.490	13.500	13.500	0	-82.055	-75.772	55.542
300	11.500	13.570	13.500	.021	-82.052	-75.732	55.170
400	11.670	16.900	13.950	1.180	-81.908	-73.647	40.238
500	11.850	19.530	14.818	2.356	-81.788	-71.601	31.296
600	12.030	21.700	15.783	3.550	-81.682	-69.570	25.340
700	12.200	23.570	16.769	4.761	-81.591	-67.555	21.091
800	12.380	25.210	17.722	5.990	-81.510	-65.556	17.909
900	12.550	26.680	18.639	7.237	-81.441	-63.567	15.436
1000	12.730	28.010	19.509	8.501	-81.379	-61.580	13.458
1100	12.910	29.230	20.336	9.783	-81.327	-59.608	11.843
1156	13.005	29.873	20.783	10.508	-81.302	-58.499	11.060
1156	13.005	29.873	20.783	10.508	-82.319	-58.499	11.060
1200	13.080	30.360	21.125	11.082	-82.254	-57.594	10.489
1300	13.260	31.420	21.882	12.399	-82.113	-55.553	9.339
1400	13.430	32.410	22.600	13.734	-81.978	-53.516	8.354
1500	13.610	33.340	23.283	15.086	-81.848	-51.482	7.501
1600	13.790	34.220	23.935	16.456	-81.725	-49.456	6.755
1700	13.960	35.060	24.564	17.843	-81.614	-47.441	6.099
1800	14.140	35.870	25.177	19.248	-81.517	-45.447	5.518
1900	14.310	36.640	25.761	20.671	-81.441	-43.446	4.997
1945	14.391	36.976	26.016	21.317	-81.417	-42.548	4.781
1945	14.391	36.976	26.016	21.317	-84.717	-42.548	4.781
2000	14.490	37.370	26.314	22.111	-84.795	-41.336	4.517

*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: $\text{Cp}^\circ = 10.970 + 1.760 \times 10^{-3}T$
 $\text{H}^\circ - \text{H}_{298}^\circ = 10.970 \times 10^{-3}T + 0.880 \times 10^{-6}T^2 - 3.349$

Reaction equations (kcal/mol):

298.15-1156 K: $\Delta \text{Hr}^\circ = -82.249 + 1.322 \times 10^{-3}T - 0.403 \times 10^{-6}T^2 - 48.950T^{-1}$
 $\Delta \text{Gr}^\circ = -82.249 - 1.322 \times 10^{-3}T \ln T + 0.403 \times 10^{-6}T^2 - 24.475T^{-1} + 29.408 \times 10^{-3}T$
1156-1945 K: $\Delta \text{Hr}^\circ = -86.286 + 3.722 \times 10^{-3}T - 0.726 \times 10^{-6}T^2 + 733.950T^{-1}$
 $\Delta \text{Gr}^\circ = -86.286 - 3.722 \times 10^{-3}T \ln T + 0.726 \times 10^{-6}T^2 + 366.975T^{-1} + 49.161 \times 10^{-3}T$
1945-2000 K: $\Delta \text{Hr}^\circ = -79.154 - 4.251 \times 10^{-3}T + 0.720 \times 10^{-6}T^2 - 34.150T^{-1}$
 $\Delta \text{Gr}^\circ = -79.154 + 4.251 \times 10^{-3}T \ln T - 0.720 \times 10^{-6}T^2 - 17.075T^{-1} - 11.972 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Pelino (97). Other data are those estimated by Mills (80).

TiS(g)
Titanium Monosulfide (ideal gas)
[Formation: $\text{Ti(c)} + \text{S(c,l)} = \text{TiS(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	8.060	58.890	58.890	0	79.800	66.709	-48.898
300	8.070	58.940	58.890	.015	79.794	66.628	-48.538
368.3	8.309	60.629	59.060	.578	79.555	63.656	-37.773
368.3	8.309	60.629	59.060	.578	79.459	63.656	-37.773
388.36	8.379	61.072	59.153	.745	79.382	62.798	-35.339
388.36	8.379	61.072	59.153	.745	78.969	62.798	-35.339
400	8.420	61.320	59.213	.843	78.906	62.314	-34.046
432.02	8.474	61.970	59.393	1.113	78.710	60.992	-30.854
500	8.590	63.220	59.832	1.694	78.177	58.246	-25.459
600	8.680	64.790	60.527	2.558	77.520	54.325	-19.788
700	8.730	66.140	61.243	3.428	76.901	50.508	-15.769
717.824	8.737	66.360	61.367	3.584	76.794	49.838	-15.174

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $C_p^\circ = 8.849 + 0.048 \times 10^{-3}T - 0.714 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 8.849 \times 10^{-3}T + 0.024 \times 10^{-6}T^2 + 0.714 \times 10^{-2}T^{-1} - 2.880$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 81.509 - 4.802 \times 10^{-3}T + 0.618 \times 10^{-6}T^2 - 99.000T^{-1}$
 $\Delta G_f^\circ = 81.509 + 4.802 \times 10^{-3}T \ln T - 0.618 \times 10^{-6}T^2 - 49.500T^{-1} - 76.259 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = 80.394 - 2.539 \times 10^{-3}T - 1.128 \times 10^{-6}T^2 + 56.600T^{-1}$
 $\Delta G_f^\circ = 80.394 + 2.539 \times 10^{-3}T \ln T + 1.128 \times 10^{-6}T^2 + 28.300T^{-1} - 61.076 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = 64.235 + 42.201 \times 10^{-3}T - 44.410 \times 10^{-6}T^2 + 1958.800T^{-1}$
 $\Delta G_f^\circ = 64.235 - 42.201 \times 10^{-3}T \ln T + 44.410 \times 10^{-6}T^2 + 979.400T^{-1} + 224.152 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = 54.757 + 38.295 \times 10^{-3}T - 24.598 \times 10^{-6}T^2 + 5185.300T^{-1}$
 $\Delta G_f^\circ = 54.757 - 38.295 \times 10^{-3}T \ln T + 24.598 \times 10^{-6}T^2 + 2592.650T^{-1} + 222.305 \times 10^{-3}T$

TiS(g)
Titanium Monosulfide (ideal gas)
[Reaction: $\text{Ti(c,l)} + 0.5\text{S}_2(\text{g}) = \text{TiS(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	8.060	58.890	58.890	0	64.445	57.195	-41.924
300	8.070	58.940	58.890	.015	64.442	57.151	-41.634
400	8.420	61.320	59.213	.843	64.255	54.748	-29.913
500	8.590	63.220	59.832	1.694	64.050	52.392	-22.900
600	8.680	64.790	60.527	2.558	63.826	50.084	-18.243
700	8.730	66.140	61.243	3.428	63.576	47.813	-14.928
800	8.770	67.310	61.930	4.304	63.304	45.578	-12.451
900	8.800	68.340	62.581	5.183	63.005	43.385	-10.535
1000	8.820	69.270	63.206	6.064	62.684	41.223	-9.009
1100	8.840	70.110	63.794	6.948	62.338	39.089	-7.766
1156	8.851	70.549	64.110	7.443	62.133	37.914	-7.168
1156	8.851	70.549	64.110	7.443	61.116	37.914	-7.168
1200	8.860	70.880	64.353	7.833	60.997	37.033	-6.745
1300	8.870	71.590	64.883	8.719	60.707	35.046	-5.892
1400	8.880	72.250	65.389	9.606	60.395	33.081	-5.164
1500	8.890	72.860	65.863	10.495	60.062	31.147	-4.538
1600	8.900	73.440	66.325	11.384	59.703	29.220	-3.991
1700	8.910	73.980	66.759	12.275	59.319	27.327	-3.513
1800	8.920	74.480	67.166	13.166	58.902	25.473	-3.093
1900	8.920	74.970	67.571	14.058	58.446	23.614	-2.716
1945	8.925	75.179	67.745	14.460	58.226	22.790	-2.561
1945	8.925	75.179	67.745	14.460	54.926	22.790	-2.561
2000	8.930	75.420	67.945	14.950	54.544	21.903	-2.393

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: $\text{Cp}^\circ = 8.849 + 0.048 \times 10^{-3}T - 0.714 \times 10^{-5}T^{-2}$
 $\text{H}^\circ - \text{H}^\circ_{298} = 8.849 \times 10^{-3}T + 0.024 \times 10^{-6}T^2 + 0.714 \times 10^{-2}T^{-1} - 2.880$

Reaction equations (kcal/mol):

298.15-1156 K: $\Delta\text{Hr}^\circ = 64.720 - 0.800 \times 10^{-3}T - 1.259 \times 10^{-6}T^2 + 22.450T^{-1}$
 $\Delta\text{Gr}^\circ = 64.720 + 0.800 \times 10^{-3}T \ln T + 1.259 \times 10^{-6}T^2 + 11.225T^{-1} - 30.296 \times 10^{-3}T$
1156-1945 K: $\Delta\text{Hr}^\circ = 60.683 + 1.600 \times 10^{-3}T - 1.582 \times 10^{-6}T^2 + 805.350T^{-1}$
 $\Delta\text{Gr}^\circ = 60.683 - 1.600 \times 10^{-3}T \ln T + 1.582 \times 10^{-6}T^2 + 402.675T^{-1} - 10.544 \times 10^{-3}T$
1945-2000 K: $\Delta\text{Hr}^\circ = 67.815 - 6.373 \times 10^{-3}T - 0.136 \times 10^{-6}T^2 + 37.250T^{-1}$
 $\Delta\text{Gr}^\circ = 67.815 + 6.373 \times 10^{-3}T \ln T + 0.136 \times 10^{-6}T^2 + 18.625T^{-1} - 71.676 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Pelino (97). Other data from Mills (80).

TiS₂(c)
Titanium Disulfide
[Formation: Ti(c) + 2S(c,l) = TiS₂(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	16.095	18.692	18.692	0	-97.300	-96.122	70.459
300	16.120	18.792	18.692	.030	-97.301	-96.114	70.018
368.3	16.666	22.166	19.031	1.155	-97.362	-95.838	56.870
368.3	16.666	22.166	19.031	1.155	-97.554	-95.838	56.870
388.36	16.827	23.055	19.217	1.491	-97.581	-95.742	53.878
388.36	16.827	23.055	19.217	1.491	-98.407	-95.742	53.878
400	16.920	23.553	19.335	1.687	-98.460	-95.662	52.267
432.02	17.054	24.861	19.697	2.231	-98.645	-95.432	48.276
500	17.340	27.377	20.575	3.401	-99.263	-94.875	41.469
600	17.730	30.572	21.982	5.154	-99.888	-93.935	34.215
700	18.220	33.339	23.410	6.950	-100.381	-92.896	29.003
717.824	18.339	33.799	23.663	7.276	-100.455	-92.703	28.224

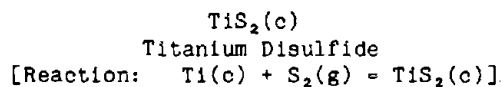
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-900 K: Cp° = 15.412 + 4.398x10⁻³T - 0.559x10⁻⁵T²
H° - H₂₉₈° = 15.412x10⁻³T + 2.199x10⁻⁶T² + 0.559x10⁻²T⁻¹ - 4.978

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -94.883 - 6.413x10⁻³T + 4.510x10⁻⁶T² - 270.100T⁻¹
ΔGf° = -94.883 + 6.413x10⁻³TlnT - 4.510x10⁻⁶T² - 135.050T⁻¹ - 37.832x10⁻³T
368.3-388.36 K: ΔHf° = -97.113 - 1.887x10⁻³T + 1.018x10⁻⁶T² + 41.100T⁻¹
ΔGf° = -97.113 + 1.887x10⁻³TlnT - 1.018x10⁻⁶T² + 20.550T⁻¹ - 7.466x10⁻³T
388.36-432.02 K: ΔHf° = -129.430 + 87.593x10⁻³T - 85.546x10⁻⁶T² + 3845.500T⁻¹
ΔGf° = -129.430 - 87.593x10⁻³TlnT + 85.546x10⁻⁶T² + 1922.750T⁻¹ + 562.991x10⁻³T
432.02-717.824 K: ΔHf° = -148.387 + 79.781x10⁻³T - 45.922x10⁻⁶T² + 10298.500T⁻¹
ΔGf° = -148.387 - 79.781x10⁻³TlnT + 45.922x10⁻⁶T² + 5149.250T⁻¹ + 559.296x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	16.095	18.692	18.692	0	-128.010	-115.150	84.406
300	16.120	18.792	18.692	.030	-128.005	-115.068	83.826
400	16.920	23.553	19.335	1.687	-127.762	-110.793	60.534
500	17.340	27.377	20.575	3.401	-127.518	-106.581	46.586
600	17.730	30.572	21.982	5.154	-127.277	-102.417	37.305
700	18.220	33.339	23.410	6.950	-127.031	-98.286	30.686
800	18.890	35.814	24.809	8.804	-126.761	-94.199	25.734
900	19.790	38.088	26.159	10.736	-126.447	-90.146	21.890

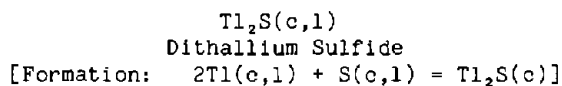
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-900 K: $C_p^\circ = 15.412 + 4.398 \times 10^{-3}T - 0.559 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 15.412 \times 10^{-3}T + 2.199 \times 10^{-6}T^2 + 0.559 \times 10^{-2}T^{-1} - 4.978$

Reaction equations (kcal/mol):

298.15-900 K: $\Delta H_r^\circ = -128.461 + 1.592 \times 10^{-3}T + 0.756 \times 10^{-6}T^2 - 27.200T^{-1}$
 $\Delta G_r^\circ = -128.461 - 1.592 \times 10^{-3}T \ln T - 0.756 \times 10^{-6}T^2 - 13.600T^{-1} + 54.094 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Mills (80). Low-temperature heat capacities and entropy at 298 K from Beyer (8). High-temperature data based on Mraw (83).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHf°	ΔGf°	
298.15	19.410	39.410	39.410	0	-22.000	-22.319	16.360
300*	19.430	39.530	39.410	.040	-21.994	-22.316	16.257
368.3	20.004	43.577	39.826	1.382	-21.905	-22.409	13.297
368.3	20.004	43.577	39.826	1.382	-22.001	-22.409	13.297
388.36	20.172	44.643	40.048	1.785	-21.978	-22.431	12.623
388.36	20.172	44.643	40.048	1.785	-22.391	-22.431	12.623
400	20.270	45.240	40.190	2.020	-22.396	-22.432	12.256
432.02	20.488	46.809	40.623	2.673	-22.431	-22.435	11.349
500	20.950	49.840	41.680	4.080	-22.627	-22.419	9.799
507	20.993	50.132	41.795	4.227	-22.644	-22.414	9.662
507	20.993	50.132	41.795	4.227	-22.824	-22.414	9.662
577	21.420	52.870	42.964	5.716	-23.019	-22.338	8.461
577	21.420	52.870	42.964	5.716	-24.999	-22.338	8.461
600	21.560	53.710	43.360	6.210	-25.022	-22.231	8.097
700	22.120	57.080	45.094	8.390	-25.062	-21.761	6.794
717.824	22.215	57.637	45.386	8.794	-25.048	-21.667	6.597

*Data above 298 K estimated except temperature and enthalpy of fusion.

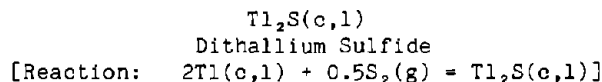
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta\text{H}^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta\text{H}^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta\text{H}^\circ = 0$ kcal/mol.
 507 K, $\alpha - \beta$ transition point of Tl; $\Delta\text{H}^\circ = 0.090$ kcal/mol.
 557 K, melting point of Tl; $\Delta\text{H}^\circ = 0.990$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-728 K: $\text{Cp}^\circ = 18.145 + 5.936 \times 10^{-3}\text{T} - 0.449 \times 10^{-5}\text{T}^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 18.145 \times 10^{-3}\text{T} + 2.968 \times 10^{-6}\text{T}^2 + 0.449 \times 10^{-2}\text{T}^{-1} - 5.824$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta\text{Hf}^\circ = -22.500 + 1.919 \times 10^{-3}\text{T} - 0.815 \times 10^{-6}\text{T}^2 + 0.100\text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -22.500 - 1.919 \times 10^{-3}\text{T} \ln \text{T} + 0.815 \times 10^{-6}\text{T}^2 + 0.050\text{T}^{-1} + 11.298 \times 10^{-3}\text{T}$
 368.3-388.36 K: $\Delta\text{Hf}^\circ = -23.615 + 4.182 \times 10^{-3}\text{T} - 2.561 \times 10^{-6}\text{T}^2 + 155.700\text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -23.615 - 4.182 \times 10^{-3}\text{T} \ln \text{T} + 2.561 \times 10^{-6}\text{T}^2 + 77.850\text{T}^{-1} + 26.481 \times 10^{-3}\text{T}$
 388.36-432.02 K: $\Delta\text{Hf}^\circ = -39.773 + 48.922 \times 10^{-3}\text{T} - 45.843 \times 10^{-6}\text{T}^2 + 2057.900\text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -39.773 - 48.922 \times 10^{-3}\text{T} \ln \text{T} + 45.843 \times 10^{-6}\text{T}^2 + 1028.950\text{T}^{-1} + 311.710 \times 10^{-3}\text{T}$
 432.02-507 K: $\Delta\text{Hf}^\circ = -49.252 + 45.016 \times 10^{-3}\text{T} - 26.031 \times 10^{-6}\text{T}^2 + 5284.400\text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -49.252 - 45.016 \times 10^{-3}\text{T} \ln \text{T} + 26.031 \times 10^{-6}\text{T}^2 + 2642.200\text{T}^{-1} + 309.862 \times 10^{-3}\text{T}$
 507-577 K: $\Delta\text{Hf}^\circ = -47.540 + 40.086 \times 10^{-3}\text{T} - 22.817 \times 10^{-6}\text{T}^2 + 5173.600\text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -47.540 - 40.086 \times 10^{-3}\text{T} \ln \text{T} + 22.817 \times 10^{-6}\text{T}^2 + 2586.800\text{T}^{-1} + 277.624 \times 10^{-3}\text{T}$
 577-717.824 K: $\Delta\text{Hf}^\circ = -49.579 + 38.868 \times 10^{-3}\text{T} - 20.531 \times 10^{-6}\text{T}^2 + 5173.600\text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -49.579 - 38.868 \times 10^{-3}\text{T} \ln \text{T} + 20.531 \times 10^{-6}\text{T}^2 + 2586.800\text{T}^{-1} + 274.732 \times 10^{-3}\text{T}$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	19.410	39.410	39.410	0	-37.355	-31.832	23.333
300*	19.430	39.530	39.410	.040	-37.346	-31.794	23.161
400	20.270	45.240	40.190	2.020	-37.047	-29.998	16.390
500	20.950	49.840	41.680	4.080	-36.755	-28.272	12.357
507	20.993	50.132	41.795	4.227	-36.737	-28.151	12.135
507	20.993	50.132	41.795	4.227	-36.917	-28.151	12.135
577	21.420	52.870	42.964	5.716	-36.807	-26.943	10.205
577	21.420	52.870	42.964	5.716	-38.787	-26.943	10.205
600	21.560	53.710	43.360	6.210	-38.716	-26.472	9.642
700	22.120	57.080	45.094	8.390	-38.387	-24.456	7.635
728	22.270	57.950	45.559	9.020	-38.276	-23.892	7.172
728	24.000	66.190	45.559	15.020	-32.276	-23.892	7.172
800	24.000	68.460	47.535	16.740	-31.893	-23.106	6.312
900	24.000	71.280	50.013	19.140	-31.353	-22.028	5.349
1000	24.000	73.810	52.270	21.540	-30.816	-21.017	4.593

*Data above 298 K estimated except temperature and enthalpy of fusion.

Phase changes: 507 K, α - β transition point of Tl; ΔH° = 0.090 kcal/mol.
577 K, melting point of Tl; ΔH° = 0.990 kcal/mol.
728 K, melting point of Tl₂S; ΔH° = 6.000 kcal/mol.

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

298.15-728 K: Cp° = 18.145 + 5.936x10⁻³T - 0.449x10⁻⁵T²
H° - H₂₉₈° = 18.145x10⁻³T + 2.968x10⁻⁶T² + 0.449x10⁻²T³ - 5.824
728-1000 K: Cp° = 24.000
H° - H₂₉₈° = 24.000x10⁻³T - 2.452

Reaction equations (kcal/mol):

298.15-507 K: ΔHr° = -39.289 + 5.922x10⁻³T - 2.692x10⁻⁶T² + 121.550T⁻¹
ΔGr° = -39.289 - 5.922x10⁻³TlnT + 2.692x10⁻⁶T² + 60.775T⁻¹ + 57.261x10⁻³T
507-577 K: ΔHr° = -37.577 + 0.991x10⁻³T + 0.522x10⁻⁶T² + 10.750T⁻¹
ΔGr° = -37.577 - 0.991x10⁻³TlnT - 0.522x10⁻⁶T² + 5.375T⁻¹ + 25.023x10⁻³T
577-728 K: ΔHr° = -39.615 - 0.226x10⁻³T + 2.808x10⁻⁶T² + 10.750T⁻¹
ΔGr° = -39.615 + 0.226x10⁻³TlnT - 2.808x10⁻⁶T² + 5.375T⁻¹ + 22.131x10⁻³T
728-1000 K: ΔHr° = -36.243 + 5.628x10⁻³T - 0.160x10⁻⁶T² - 34.150T⁻¹
ΔGr° = -36.243 - 5.628x10⁻³TlnT + 0.160x10⁻⁶T² - 17.075T⁻¹ + 53.967x10⁻³T

Sources: Enthalpy of formation at 298 K based on Maekawa (72). Low-temperature heat capacities and entropy at 298 K from Guseinov (51). Data extrapolated 300-728 K. Enthalpy of fusion from Tkachenko (118). Heat capacity of liquid estimated.

TmS(g)
Thulium Monosulfide (ideal gas)
[Formation: Tm(c) + S(c,l) = TmS(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	8.200	61.810	61.810	0	38.500	27.630	-20.253
300	8.210	61.860	61.810	.015	38.493	27.562	-20.079
368.3	8.415	63.571	61.984	.585	38.236	25.099	-14.893
368.3	8.415	63.571	61.984	.585	38.140	25.099	-14.893
388.36	8.475	64.019	62.077	.754	38.061	24.391	-13.726
388.36	8.475	64.019	62.077	.754	37.648	24.391	-13.726
400	8.510	64.270	62.137	.853	37.583	23.995	-13.110
432.02	8.555	64.927	62.320	1.126	37.385	22.914	-11.592
500	8.650	66.180	62.756	1.712	36.855	20.684	-9.041
600	8.730	67.770	63.468	2.581	36.214	17.507	-6.377
700	8.780	69.120	64.183	3.456	35.623	14.438	-4.508
717.824	8.785	69.341	64.308	3.613	35.522	13.901	-4.232

*Data except enthalpy of formation at 298 K estimated.

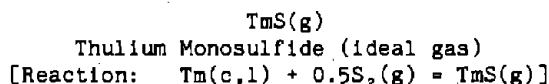
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 8.875 + 0.036x10⁻³T - 0.608x10⁻⁵T⁻²
H° - H°₂₉₈ = 8.875x10⁻³T + 0.018x10⁻⁶T² + 0.608x10⁻²T⁻¹ - 2.852

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 39.977 - 4.620x10⁻³T + 0.701x10⁻⁶T² - 48.400T⁻¹
ΔGf° = 39.977 + 4.620x10⁻³TlnT - 0.701x10⁻⁶T² - 24.200T⁻¹ - 67.256x10⁻³T
368.3-388.36 K: ΔHf° = 38.862 - 2.357x10⁻³T - 1.045x10⁻⁶T² + 107.200T⁻¹
ΔGf° = 38.862 + 2.357x10⁻³TlnT + 1.045x10⁻⁶T² + 53.600T⁻¹ - 52.073x10⁻³T
388.36-432.02 K: ΔHf° = 22.704 + 42.383x10⁻³T - 44.327x10⁻⁶T² + 2009.400T⁻¹
ΔGf° = 22.704 - 42.383x10⁻³TlnT + 44.327x10⁻⁶T² + 1004.700T⁻¹ + 233.155x10⁻³T
432.02-717.824 K: ΔHf° = 13.225 + 38.477x10⁻³T - 24.515x10⁻⁶T² + 5235.900T⁻¹
ΔGf° = 13.225 - 38.477x10⁻³TlnT + 24.515x10⁻⁶T² + 2617.950T⁻¹ + 231.308x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H° ₂₉₈)/T	H°- H° ₂₉₈	ΔHr°	ΔGr°	
298.15*	8.200	61.810	61.810	0	23.145	18.116	-13.279
300	8.210	61.860	61.810	.015	23.141	18.085	-13.175
400	8.510	64.270	62.137	.853	22.932	16.429	-8.976
500	8.650	66.180	62.756	1.712	22.728	14.830	-6.482
600	8.730	67.770	63.468	2.581	22.520	13.266	-4.832
700	8.780	69.120	64.183	3.456	22.298	11.743	-3.666
800	8.810	70.290	64.870	4.336	22.050	10.253	-2.801
900	8.830	71.330	65.532	5.218	21.772	8.795	-2.136
1000	8.850	72.260	66.158	6.102	21.468	7.376	-1.612
1100	8.860	73.110	66.757	6.988	21.144	5.970	-1.186
1200	8.880	73.880	67.317	7.875	20.800	4.610	-.839
1300	8.890	74.590	67.849	8.763	20.436	3.277	-.551
1400	8.890	75.250	68.356	9.652	20.051	1.978	-.309
1500	8.900	75.860	68.832	10.542	19.644	.699	-.102
1600	8.910	76.440	69.295	11.432	19.217	-.559	.076
1700	8.910	76.980	69.731	12.323	18.770	-1.776	.228
1800	8.920	77.490	70.148	13.215	18.305	-2.981	.362
1818	8.922	77.579	70.221	13.376	18.219	-3.186	.383
1818	8.922	77.579	70.221	13.376	14.194	-3.186	.383
1900	8.930	77.970	70.545	14.108	13.725	-3.961	.456
2000	8.930	78.430	70.930	15.000	13.149	-4.877	.533

*Data except enthalpy of formation at 298 K estimated.

Phase change: 1818 K, melting point of Tm; ΔH° = 4.025 kcal/mol.

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

$$298.15-2000 \text{ K: } \begin{aligned} \text{Cp}^\circ &= 8.875 + 0.036 \times 10^{-3} T - 0.608 \times 10^{-5} T^2 \\ \text{H}^\circ - \text{H}_{298}^\circ &= 8.875 \times 10^{-3} T + 0.018 \times 10^{-6} T^2 + 0.608 \times 10^{-2} T^{-1} - 2.852 \end{aligned}$$

Reaction equations (kcal/mol):

$$\begin{aligned} 298.15-1818 \text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= 23.189 - 0.618 \times 10^{-3} T - 1.176 \times 10^{-6} T^2 + 73.050 T^{-1} \\ \Delta \text{Gr}^\circ &= 23.189 + 0.618 \times 10^{-3} T \ln T + 1.176 \times 10^{-6} T^2 + 36.525 T^{-1} - 21.293 \times 10^{-3} T \end{aligned} \\ 1818-2000 \text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= 24.078 - 5.187 \times 10^{-3} T - 0.142 \times 10^{-6} T^2 + 26.650 T^{-1} \\ \Delta \text{Gr}^\circ &= 24.078 + 5.187 \times 10^{-3} T \ln T + 0.142 \times 10^{-6} T^2 + 13.325 T^{-1} - 54.188 \times 10^{-3} T \end{aligned} \end{aligned}$$

Source: Data from Mills (80) who estimated all except enthalpy of formation at 298 K.

US(c)
Uranium Monosulfide
[Formation: $U(c) + S(c,1) = US(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	12.080	18.640	18.640	0	-77.000	-76.696	56.219
300	12.100	18.715	18.642	.022	-77.000	-76.694	55.871
368.3	12.510	21.242	18.895	.864	-77.005	-76.625	45.469
368.3	12.510	21.242	18.895	.864	-77.101	-76.625	45.469
388.36	12.630	21.909	19.034	1.117	-77.108	-76.598	43.105
388.36	12.630	21.909	19.034	1.117	-77.521	-76.598	43.105
400	12.700	22.283	19.123	1.264	-77.544	-76.570	41.835
432.02	12.818	23.266	19.394	1.673	-77.628	-76.489	38.694
500	13.070	25.159	20.051	2.554	-77.927	-76.283	33.343
600	13.340	27.567	21.109	3.875	-78.260	-75.922	27.654
700	13.560	29.640	22.183	5.220	-78.583	-75.506	23.574
717.824	13.596	29.981	22.372	5.462	-78.641	-75.427	22.964

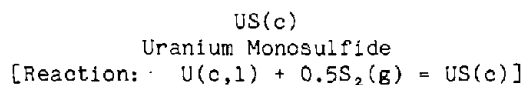
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $C_p^\circ = 12.685 + 1.518 \times 10^{-3}T - 0.940 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 12.685 \times 10^{-3}T + 0.759 \times 10^{-6}T^2 + 0.940 \times 10^{-2}T^{-1} - 4.165$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -77.349 + 1.401 \times 10^{-3}T - 1.746 \times 10^{-6}T^2 + 25.900T^{-1}$
 $\Delta G_f^\circ = -77.349 - 1.401 \times 10^{-3}T \ln T + 1.746 \times 10^{-6}T^2 + 12.950T^{-1} + 9.509 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -78.464 + 3.664 \times 10^{-3}T - 3.492 \times 10^{-6}T^2 + 181.500T^{-1}$
 $\Delta G_f^\circ = -78.464 - 3.664 \times 10^{-3}T \ln T + 3.492 \times 10^{-6}T^2 + 90.750T^{-1} + 24.692 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -94.623 + 48.404 \times 10^{-3}T - 46.774 \times 10^{-6}T^2 + 2083.700T^{-1}$
 $\Delta G_f^\circ = -94.623 - 48.404 \times 10^{-3}T \ln T + 46.774 \times 10^{-6}T^2 + 1041.850T^{-1} + 309.920 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = -104.101 + 44.498 \times 10^{-3}T - 26.962 \times 10^{-6}T^2 + 5310.200T^{-1}$
 $\Delta G_f^\circ = -104.101 - 44.498 \times 10^{-3}T \ln T + 26.962 \times 10^{-6}T^2 + 2655.100T^{-1} + 308.073 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	12.080	18.640	18.640	0	-92.355	-86.209	63.192
300	12.100	18.715	18.642	.022	-92.352	-86.171	62.775
400	12.700	22.283	19.123	1.264	-92.195	-84.136	45.969
500	13.070	25.159	20.051	2.554	-92.054	-82.136	35.901
600	13.340	27.567	21.109	3.875	-91.954	-80.163	29.199
700	13.560	29.640	22.183	5.220	-91.908	-78.202	24.415
800	13.760	31.464	23.232	6.586	-91.931	-76.244	20.829
900	13.940	33.095	24.238	7.971	-92.035	-74.278	18.037
942	14.011	33.732	24.648	8.558	-92.106	-73.448	17.040
942	14.011	33.732	24.648	8.558	-92.773	-73.448	17.040
1000	14.110	34.572	25.198	9.374	-92.810	-72.255	15.791
1049	14.188	35.249	25.652	10.067	-92.837	-71.247	14.843
1049	14.188	35.249	25.652	10.067	-93.974	-71.247	14.843
1100	14.270	35.925	26.114	10.792	-93.946	-70.145	13.936
1200	14.440	37.174	26.984	12.228	-93.876	-67.984	12.381
1300	14.600	38.336	27.813	13.680	-93.793	-65.830	11.067
1400	14.760	39.424	28.604	15.148	-93.699	-63.681	9.941
1408	14.773	39.508	28.666	15.266	-93.690	-63.510	9.858
1408	14.773	39.508	28.666	15.266	-95.875	-63.510	9.858
1500	14.920	40.447	29.359	16.632	-96.005	-61.390	8.944
1600	15.080	41.415	30.083	18.132	-96.133	-59.079	8.070
1700	15.240	42.334	30.776	19.648	-96.250	-56.759	7.297
1800	15.400	43.210	31.443	21.180	-96.353	-54.433	6.609
1900	15.560	44.047	32.085	22.728	-96.443	-52.102	5.993
2000	15.720	44.849	32.703	24.292	-96.521	-49.766	5.438

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:

298.15-2000 K: $\text{Cp}^\circ = 12.685 + 1.518 \times 10^{-3}T - 0.940 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 12.685 \times 10^{-3}T + 0.759 \times 10^{-6}T^2 + 0.940 \times 10^{-2}T^{-1} - 4.165$

Reaction equations (kcal/mol):

298.15-942 K: $\Delta\text{Hr}^\circ = -94.138 + 5.404 \times 10^{-3}T - 3.623 \times 10^{-6}T^2 + 147.350T^{-1}$
 $\Delta\text{Gr}^\circ = -94.138 - 5.404 \times 10^{-3}T \ln T + 3.623 \times 10^{-6}T^2 + 73.675T^{-1} + 55.472 \times 10^{-3}T$
942-1049 K: $\Delta\text{Hr}^\circ = -91.728 - 1.742 \times 10^{-3}T + 0.599 \times 10^{-6}T^2 + 59.850T^{-1}$
 $\Delta\text{Gr}^\circ = -91.728 + 1.742 \times 10^{-3}T \ln T - 0.599 \times 10^{-6}T^2 + 29.925T^{-1} + 8.011 \times 10^{-3}T$
1049-1408 K: $\Delta\text{Hr}^\circ = -94.024 - 0.636 \times 10^{-3}T + 0.599 \times 10^{-6}T^2 + 59.850T^{-1}$
 $\Delta\text{Gr}^\circ = -94.024 + 0.636 \times 10^{-3}T \ln T - 0.599 \times 10^{-6}T^2 + 29.925T^{-1} + 17.886 \times 10^{-3}T$
1408-2000 K: $\Delta\text{Hr}^\circ = -92.717 - 3.117 \times 10^{-3}T + 0.599 \times 10^{-6}T^2 + 59.850T^{-1}$
 $\Delta\text{Gr}^\circ = -92.717 + 3.117 \times 10^{-3}T \ln T - 0.599 \times 10^{-6}T^2 + 29.925T^{-1} - 1.022 \times 10^{-3}T$

Source: Data from Gronvold (47).

US(g)
 Uranium Monosulfide (ideal gas)
 [Formation: $\text{U(c)} + \text{S(c,l)} = \text{US(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	8.410	62.670	62.670	0	74.200	61.377	-44.990
300	8.417	62.722	62.670	.016	74.194	61.298	-44.655
368.3	8.656	64.474	62.848	.599	73.929	58.388	-34.647
368.3	8.656	64.474	62.848	.599	73.833	58.388	-34.647
388.36	8.726	64.935	62.944	.773	73.748	57.549	-32.385
388.36	8.726	64.935	62.944	.773	73.335	57.549	-32.385
400	8.767	65.193	63.006	.875	73.267	57.077	-31.185
432.02	8.857	65.872	63.193	1.157	73.056	55.789	-28.222
500	9.049	67.181	63.647	1.767	72.486	53.119	-23.218
600	9.281	68.852	64.380	2.683	71.748	49.315	-17.963
700	9.470	70.297	65.124	3.621	71.018	45.635	-14.248
717.824	9.497	70.535	65.256	3.790	70.887	44.991	-13.698

*Data except enthalpy of formation at 298 K estimated.

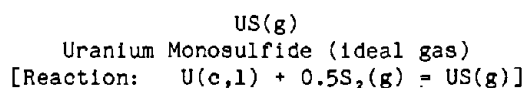
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $\text{Cp}^\circ = 9.169 + 0.630 \times 10^{-3}T - 0.842 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 9.169 \times 10^{-3}T + 0.315 \times 10^{-6}T^2 + 0.842 \times 10^{-2}T^{-1} - 3.044$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 74.971 - 2.115 \times 10^{-3}T - 2.190 \times 10^{-6}T^2 + 16.100T^{-1}$
 $\Delta G_f^\circ = 74.971 + 2.115 \times 10^{-3}T \ln T + 2.190 \times 10^{-6}T^2 + 8.050T^{-1} - 58.390 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = 73.856 + 0.148 \times 10^{-3}T - 3.936 \times 10^{-6}T^2 + 171.700T^{-1}$
 $\Delta G_f^\circ = 73.856 - 0.148 \times 10^{-3}T \ln T + 3.936 \times 10^{-6}T^2 + 85.850T^{-1} - 43.207 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = 57.698 + 44.888 \times 10^{-3}T - 47.218 \times 10^{-6}T^2 + 2073.900T^{-1}$
 $\Delta G_f^\circ = 57.698 - 44.888 \times 10^{-3}T \ln T + 47.218 \times 10^{-6}T^2 + 1036.950T^{-1} + 242.022 \times 10^{-3}T$
 432.02-717.824 K: $\Delta H_f^\circ = 48.219 + 40.982 \times 10^{-3}T - 27.406 \times 10^{-6}T^2 + 5300.400T^{-1}$
 $\Delta G_f^\circ = 48.219 - 40.982 \times 10^{-3}T \ln T + 27.406 \times 10^{-6}T^2 + 2650.200T^{-1} + 240.174 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15*	8.410	62.670	62.670	0	58.845	51.863	-38.016
300	8.417	62.722	62.670	.016	58.842	51.821	-37.751
400	8.767	65.193	63.006	.875	58.616	49.511	-27.051
500	9.049	67.181	63.647	1.767	58.358	47.266	-20.660
600	9.281	68.852	64.380	2.683	58.053	45.074	-16.418
700	9.470	70.297	65.124	3.621	57.693	42.939	-13.406
800	9.623	71.572	65.852	4.576	57.260	40.860	-11.162
900	9.746	72.713	66.552	5.545	56.739	38.840	-9.432
942	9.787	73.158	66.837	5.955	56.491	38.010	-8.818
942	9.787	73.158	66.837	5.955	55.824	38.010	-8.818
1000	9.843	73.745	67.221	6.524	55.540	36.921	-8.069
1049	9.880	74.217	67.537	7.007	55.302	36.016	-7.504
1049	9.880	74.217	67.537	7.007	54.165	36.016	-7.504
1100	9.918	74.686	67.856	7.513	53.975	35.139	-6.981
1200	9.973	75.552	68.463	8.507	53.604	33.442	-6.090
1300	10.012	76.352	69.039	9.507	53.234	31.776	-5.342
1400	10.037	77.095	69.589	10.509	52.862	30.140	-4.705
1408	10.038	77.152	69.631	10.589	52.833	30.011	-4.658
1408	10.038	77.152	69.631	10.589	50.648	30.011	-4.658
1500	10.049	77.786	70.110	11.514	50.077	28.684	-4.179
1600	10.051	78.436	70.612	12.519	49.454	27.275	-3.726
1700	10.045	79.045	71.090	13.524	48.826	25.908	-3.331
1800	10.032	79.619	71.548	14.527	48.194	24.578	-2.984
1900	10.013	80.161	71.987	15.530	47.559	23.284	-2.678
2000	9.991	80.674	72.409	16.530	46.917	22.021	-2.406

*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:

298.15-2000 K: $\text{Cp}^\circ = 9.169 + 0.630 \times 10^{-3}T - 0.842 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 9.169 \times 10^{-3}T + 0.315 \times 10^{-6}T^2 + 0.842 \times 10^{-2}T^{-1} - 3.044$

Reaction equations (kcal/mol):

298.15-942 K: $\Delta\text{Hr}^\circ = 58.182 + 1.887 \times 10^{-3}T - 4.067 \times 10^{-6}T^2 + 137.550T^{-1}$
 $\Delta\text{Gr}^\circ = 58.182 - 1.887 \times 10^{-3}T \ln T + 4.067 \times 10^{-6}T^2 + 68.775T^{-1} - 12.427 \times 10^{-3}T$
 942-1049 K: $\Delta\text{Hr}^\circ = 60.592 - 5.258 \times 10^{-3}T + 0.155 \times 10^{-6}T^2 + 50.050T^{-1}$
 $\Delta\text{Gr}^\circ = 60.592 + 5.258 \times 10^{-3}T \ln T - 0.155 \times 10^{-6}T^2 + 25.025T^{-1} - 59.888 \times 10^{-3}T$
 1049-1408 K: $\Delta\text{Hr}^\circ = 58.296 - 4.153 \times 10^{-3}T + 0.155 \times 10^{-6}T^2 + 50.050T^{-1}$
 $\Delta\text{Gr}^\circ = 58.296 + 4.153 \times 10^{-3}T \ln T - 0.155 \times 10^{-6}T^2 + 25.025T^{-1} - 50.013 \times 10^{-3}T$
 1408-2000 K: $\Delta\text{Hr}^\circ = 59.603 - 6.633 \times 10^{-3}T + 0.155 \times 10^{-6}T^2 + 50.050T^{-1}$
 $\Delta\text{Gr}^\circ = 59.603 + 6.633 \times 10^{-3}T \ln T - 0.155 \times 10^{-6}T^2 + 25.025T^{-1} - 68.921 \times 10^{-3}T$

Source: Data from Gronvold (47) who estimated all except enthalpy of formation at 298 K.

(US)₂(g)
 Dimeric Uranium Monosulfide (ideal gas)
 [Formation: 2U(c) + 2S(c,l) = (US)₂(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	18.765	90.300	90.300	0	43.000	27.801	-20.378
300	18.777	90.416	90.300	.035	42.991	27.708	-20.185
368.3	19.088	94.304	90.694	1.330	42.591	24.267	-14.400
368.3	19.088	94.304	90.694	1.330	42.399	24.267	-14.400
388.36	19.180	95.319	90.907	1.713	42.264	23.284	-13.103
388.36	19.180	95.319	90.907	1.713	41.438	23.284	-13.103
400	19.233	95.886	91.044	1.937	41.321	22.741	-12.425
432.02	19.304	97.370	91.458	2.554	40.952	21.267	-10.758
500	19.456	100.203	92.459	3.872	39.910	18.256	-7.979
600	19.580	103.762	94.054	5.825	38.555	14.053	-5.119
700	19.656	106.787	95.663	7.787	37.181	10.079	-3.147
717.824	19.665	107.281	95.945	8.137	36.931	9.393	-2.860

*Data estimated.

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 19.813 + 0.038x10⁻³T - 0.942x10⁻⁵T⁻²
 H° - H°₂₉₈ = 19.813x10⁻³T + 0.019x10⁻⁶T² + 0.942x10⁻²T⁻¹ - 6.225

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 44.406 - 2.755x10⁻³T - 4.991x10⁻⁶T² - 42.000T⁻¹
 ΔGf° = 44.406 + 2.755x10⁻³TlnT + 4.991x10⁻⁶T² - 21.000T⁻¹ - 72.642x10⁻³T
 368.3-388.36 K: ΔHf° = 42.176 + 1.771x10⁻³T - 8.483x10⁻⁶T² + 269.200T⁻¹
 ΔGf° = 42.176 - 1.771x10⁻³TlnT + 8.483x10⁻⁶T² + 134.600T⁻¹ - 42.276x10⁻³T
 388.36-432.02 K: ΔHf° = 9.859 + 91.251x10⁻³T - 95.047x10⁻⁶T² + 4073.600T⁻¹
 ΔGf° = 9.859 - 91.251x10⁻³TlnT + 95.047x10⁻⁶T² + 2036.800T⁻¹ + 528.180x10⁻³T
 432.02-717.824 K: ΔHf° = -9.098 + 83.439x10⁻³T - 55.423x10⁻⁶T² + 10526.600T⁻¹
 ΔGf° = -9.098 - 83.439x10⁻³TlnT + 55.423x10⁻⁶T² + 5263.300T⁻¹ + 524.485x10⁻³T

(US)₂(g)
 Dimeric Uranium Monosulfide (ideal gas)
 [Reaction: 2U(c,l) + S₂(g) = (US)₂(g)]

T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	18.765	90.300	90.300	0	12.290	8.774	-6.431
300	18.777	90.416	90.300	.035	12.287	8.753	-6.377
400	19.233	95.886	91.044	1.937	12.019	7.610	-4.158
500	19.456	100.203	92.459	3.872	11.655	6.549	-2.863
600	19.580	103.762	94.054	5.825	11.166	5.572	-2.029
700	19.656	106.787	95.663	7.787	10.531	4.689	-1.464
800	19.706	109.415	97.221	9.755	9.722	3.906	-1.067
900	19.741	111.738	98.708	11.727	8.716	3.237	-.786
942	19.751	112.639	99.309	12.556	8.228	2.991	-.694
942	19.751	112.639	99.309	12.556	6.894	2.991	-.694
1000	19.765	113.819	100.116	13.703	6.335	2.769	-.605
1049	19.774	114.765	100.778	14.672	5.862	2.608	-.543
1049	19.774	114.765	100.778	14.672	3.588	2.608	-.543
1100	19.784	115.704	101.449	15.680	3.205	2.567	-.510
1200	19.798	117.426	102.710	17.659	2.452	2.542	-.463
1300	19.809	119.011	103.903	19.640	1.694	2.579	-.434
1400	19.817	120.479	105.035	21.621	.928	2.679	-.418
1408	19.818	120.592	105.123	21.780	.867	2.690	-.418
1408	19.818	120.592	105.123	21.780	-3.503	2.690	-.418
1500	19.824	121.847	106.112	23.603	-4.670	3.130	-.456
1600	19.830	123.127	107.136	25.586	-5.944	3.690	-.504
1700	19.835	124.329	108.112	27.569	-7.226	4.331	-.557
1800	19.839	125.463	109.045	29.553	-8.512	5.049	-.613
1900	19.842	126.535	109.937	31.537	-9.805	5.840	-.672
2000	19.845	127.553	110.793	33.521	-11.104	6.694	-.731

*Data 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:

298.15-2000 K: Cp° = 19.813 + 0.038x10⁻³T - 0.942x10⁻⁵T⁻²
 H° - H₂₉₈° = 19.813x10⁻³T + 0.019x10⁻⁶T² + 0.942x10⁻²T⁻¹ - 6.225

Reaction equations (kcal/mol):

298.15-942 K: ΔHr° = 10.828 + 5.250x10⁻³T - 8.745x10⁻⁶T² + 200.900T⁻¹
 ΔGr° = 10.828 - 5.250x10⁻³TlnT + 8.745x10⁻⁶T² + 100.450T⁻¹ + 19.284x10⁻³T
 942-1049 K: ΔHr° = 15.648 - 9.040x10⁻³T - 0.301x10⁻⁶T² + 25.900T⁻¹
 ΔGr° = 15.648 + 9.040x10⁻³TlnT + 0.301x10⁻⁶T² + 12.950T⁻¹ - 75.638x10⁻³T
 1049-1408 K: ΔHr° = 11.056 - 6.830x10⁻³T - 0.301x10⁻⁶T² + 25.900T⁻¹
 ΔGr° = 11.056 + 6.830x10⁻³TlnT + 0.301x10⁻⁶T² + 12.950T⁻¹ - 55.889x10⁻³T
 1408-2000 K: ΔHr° = 13.670 - 11.790x10⁻³T - 0.301x10⁻⁶T² + 25.900T⁻¹
 ΔGr° = 13.670 + 11.790x10⁻³TlnT + 0.301x10⁻⁶T² + 12.950T⁻¹ - 93.705x10⁻³T

Source: Data are those estimated by Gronvold (47).

US_{1.5}(c)
 Uranium Sesquisulfide
 [Formation: U(c) + 1.5S(c,l) = US_{1.5}(c)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	15.980	23.800	23.800	0	-105.000	-105.092	77.034
300*	16.000	23.899	23.800	.030	-104.997	-105.092	76.558
368.3	16.123	27.193	24.133	1.127	-104.939	-105.122	62.379
368.3	16.123	27.193	24.133	1.127	-105.083	-105.122	62.379
388.36	16.159	28.049	24.314	1.451	-105.078	-105.123	59.157
388.36	16.159	28.049	24.314	1.451	-105.698	-105.123	59.157
400	16.180	28.527	24.430	1.639	-105.724	-105.106	57.426
432.02	16.234	29.775	24.780	2.158	-105.830	-105.053	53.144
500	16.350	32.155	25.625	3.265	-106.240	-104.894	45.849
600	16.520	35.151	26.969	4.909	-106.678	-104.582	38.094
700	16.700	37.711	28.325	6.570	-107.085	-104.200	32.532
717.824	16.730	38.131	28.564	6.868	-107.156	-104.124	31.702

*Data above 298 K estimated.

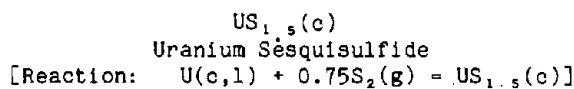
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 15.494 + 1.736x10⁻³T - 0.028x10⁻⁵T⁻²
 H° - H₂₉₈° = 15.494x10⁻³T + 0.868x10⁻⁶T² + 0.028x10⁻²T⁻¹ - 4.706

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -104.488 + 0.123x10⁻³T - 0.778x10⁻⁶T² - 143.100T⁻¹
 ΔGf° = -104.488 - 0.123x10⁻³TlnT + 0.778x10⁻⁶T² - 71.550T⁻¹ - 0.754x10⁻³T
 368.3-388.36 K: ΔHf° = -106.160 + 3.518x10⁻³T - 3.398x10⁻⁶T² + 90.300T⁻¹
 ΔGf° = -106.160 - 3.518x10⁻³TlnT + 3.398x10⁻⁶T² + 45.150T⁻¹ + 22.021x10⁻³T
 388.36-432.02 K: ΔHf° = -130.398 + 70.628x10⁻³T - 68.321x10⁻⁶T² + 2943.600T⁻¹
 ΔGf° = -130.398 - 70.628x10⁻³TlnT + 68.321x10⁻⁶T² + 1471.800T⁻¹ + 449.863x10⁻³T
 432.02-717.824 K: ΔHf° = -144.616 + 64.769x10⁻³T - 38.603x10⁻⁶T² + 7783.350T⁻¹
 ΔGf° = -144.616 - 64.769x10⁻³TlnT + 38.603x10⁻⁶T² + 3891.675T⁻¹ + 447.092x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr.
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔH°	ΔG°	
298.15	15.980	23.800	23.800	0	-128.033	-119.362	87.494
300*	16.000	23.899	23.800	.030	-128.025	-119.308	86.914
400	16.180	28.527	24.430	1.639	-127.701	-116.454	63.627
500	16.350	32.155	25.625	3.265	-127.431	-113.674	49.686
600	16.520	35.151	26.969	4.909	-127.220	-110.944	40.411
700	16.700	37.711	28.325	6.570	-127.073	-108.242	33.794
800	16.870	39.952	29.642	8.248	-127.001	-105.559	28.837
900	17.050	41.950	30.901	9.944	-127.014	-102.880	24.982
942	17.126	42.729	31.411	10.662	-127.048	-101.753	23.607
942	17.126	42.729	31.411	10.662	-127.715	-101.753	23.607
1000	17.230	43.756	32.098	11.658	-127.700	-100.155	21.889
1049	17.313	44.582	32.662	12.504	-127.684	-98.805	20.585
1049	17.313	44.582	32.662	12.504	-128.821	-98.805	20.585
1100	17.400	45.406	33.233	13.390	-128.745	-97.347	19.341
1200	17.570	46.927	34.312	15.138	-128.589	-94.500	17.211
1300	17.750	48.341	35.338	16.904	-128.420	-91.668	15.411
1400	17.920	49.662	36.313	18.688	-128.238	-88.844	13.869
1408	17.934	49.764	36.390	18.831	-128.223	-88.619	13.755
1408	17.934	49.764	36.390	18.831	-130.408	-88.619	13.755
1500	18.100	50.905	37.246	20.489	-130.458	-85.888	12.514
1600	18.270	52.078	38.136	22.307	-130.502	-82.916	11.326
1700	18.450	53.191	38.989	24.143	-130.533	-79.941	10.277
1800	18.620	54.251	39.809	25.996	-130.551	-76.965	9.345
1900	18.810	55.262	40.595	27.868	-130.555	-73.986	8.510
2000	19.000	56.232	41.353	29.758	-130.546	-71.011	7.760

*Data above 298 K estimated.

Phase changes: 942 K, $\alpha - \beta$ transition point of U; $\Delta\text{H}^\circ = 0.667$ kcal/mol.
 1049 K, $\beta - \gamma$ transition point of U; $\Delta\text{H}^\circ = 1.137$ kcal/mol.
 1408 K, melting point of U; $\Delta\text{H}^\circ = 2.185$ kcal/mol.

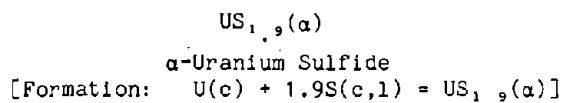
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $\text{Cp}^\circ = 15.494 + 1.736 \times 10^{-3}T - 0.028 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 15.494 \times 10^{-3}T + 0.868 \times 10^{-6}T^2 + 0.028 \times 10^{-2}T^3 - 4.706$

Reaction equations (kcal/mol):

298.15-942 K: $\Delta\text{H}^\circ = -129.671 + 6.127 \times 10^{-3}T - 3.594 \times 10^{-6}T^2 + 39.075T^{-1}$
 $\Delta\text{G}^\circ = -129.671 - 6.127 \times 10^{-3}T \ln T + 3.594 \times 10^{-6}T^2 + 19.538T^{-1} + 68.191 \times 10^{-3}T$
 942-1049 K: $\Delta\text{H}^\circ = -127.261 - 1.018 \times 10^{-3}T + 0.628 \times 10^{-6}T^2 - 48.425T^{-1}$
 $\Delta\text{G}^\circ = -127.261 + 1.018 \times 10^{-3}T \ln T - 0.628 \times 10^{-6}T^2 - 24.212T^{-1} + 20.730 \times 10^{-3}T$
 1049-1408 K: $\Delta\text{H}^\circ = -129.557 + 0.087 \times 10^{-3}T + 0.628 \times 10^{-6}T^2 - 48.425T^{-1}$
 $\Delta\text{G}^\circ = -129.557 - 0.087 \times 10^{-3}T \ln T - 0.628 \times 10^{-6}T^2 - 24.212T^{-1} + 30.605 \times 10^{-3}T$
 1408-2000 K: $\Delta\text{H}^\circ = -128.250 - 2.393 \times 10^{-3}T + 0.628 \times 10^{-6}T^2 - 48.425T^{-1}$
 $\Delta\text{G}^\circ = -128.250 + 2.393 \times 10^{-3}T \ln T - 0.628 \times 10^{-6}T^2 - 24.212T^{-1} + 11.697 \times 10^{-3}T$

Source: Data from Gronvold (47) who estimated all above 298 K.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHf°	ΔGf°	
298.15*	17.680	26.210	26.210	0	-123.000	-122.897	90.085
300	17.700	26.319	26.210	.033	-122.998	-122.895	89.528
368.3	18.246	30.012	26.581	1.264	-122.960	-122.878	72.915
368.3	18.246	30.012	26.581	1.264	-123.143	-122.878	72.915
388.36	18.407	30.984	26.784	1.631	-123.142	-122.862	69.140
388.36	18.407	30.984	26.784	1.631	-123.926	-122.862	69.140
400	18.500	31.529	26.914	1.846	-123.961	-122.830	67.110
432.02	18.644	32.959	27.310	2.441	-124.096	-122.736	62.089
500	18.950	35.708	28.270	3.719	-124.604	-122.476	53.534
600	19.260	39.192	29.809	5.630	-125.119	-122.001	44.438
700	19.510	42.180	31.367	7.569	-125.568	-121.444	37.916
717.824	19.547	42.671	31.642	7.917	-125.643	-121.337	36.942

*Enthalpy of formation at 298 K and data above 298 K estimated.

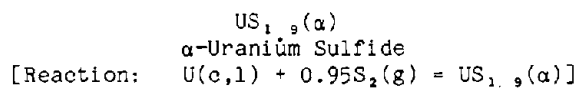
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta\text{H}^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta\text{H}^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta\text{H}^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-1900 K: $\text{Cp}^\circ = 18.652 + 1.586 \times 10^{-3}\text{T} - 1.284 \times 10^{-5}\text{T}^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 18.652 \times 10^{-3}\text{T} + 0.793 \times 10^{-6}\text{T}^2 + 1.284 \times 10^{-2}\text{T}^{-1} - 6.062$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta\text{Hf}^\circ = -122.721 + 0.011 \times 10^{-3}\text{T} - 0.167 \times 10^{-6}\text{T}^2 - 79.740\text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -122.721 - 0.011 \times 10^{-3}\text{T} \ln \text{T} + 0.167 \times 10^{-6}\text{T}^2 - 39.870\text{T}^{-1} - 0.126 \times 10^{-3}\text{T}$
 368.3-388.36 K: $\Delta\text{Hf}^\circ = -124.840 + 4.311 \times 10^{-3}\text{T} - 3.484 \times 10^{-6}\text{T}^2 + 215.900\text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -124.840 - 4.311 \times 10^{-3}\text{T} \ln \text{T} + 3.484 \times 10^{-6}\text{T}^2 + 107.950\text{T}^{-1} + 28.722 \times 10^{-3}\text{T}$
 388.36-432.02 K: $\Delta\text{Hf}^\circ = -155.541 + 89.317 \times 10^{-3}\text{T} - 85.720 \times 10^{-6}\text{T}^2 + 3830.080\text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -155.541 - 89.317 \times 10^{-3}\text{T} \ln \text{T} + 85.720 \times 10^{-6}\text{T}^2 + 1915.040\text{T}^{-1} + 570.656 \times 10^{-3}\text{T}$
 432.02-717.824 K: $\Delta\text{Hf}^\circ = -173.550 + 81.896 \times 10^{-3}\text{T} - 48.077 \times 10^{-6}\text{T}^2 + 9960.431\text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -173.550 - 81.896 \times 10^{-3}\text{T} \ln \text{T} + 48.077 \times 10^{-6}\text{T}^2 + 4980.215\text{T}^{-1} + 567.146 \times 10^{-3}\text{T}$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHr°	ΔGr°	
298.15*	17.680	26.210	26.210	0	-152.174	-140.973	103.335
300	17.700	26.319	26.210	.033	-152.167	-140.902	102.646
400	18.500	31.529	26.914	1.846	-151.798	-137.205	74.964
500	18.950	35.708	28.270	3.719	-151.447	-133.597	58.395
600	19.260	39.192	29.809	5.630	-151.138	-130.058	47.373
700	19.510	42.180	31.367	7.569	-150.885	-126.564	39.515
800	19.720	44.799	32.885	9.531	-150.704	-123.103	33.630
900	19.920	47.133	34.341	11.513	-150.607	-119.660	29.057
942	19.996	48.043	34.932	12.351	-150.594	-118.217	27.427
942	19.996	48.043	34.932	12.351	-151.261	-118.217	27.427
1000	20.100	49.242	35.728	13.514	-151.183	-116.185	25.392
1049	20.188	50.206	36.382	14.501	-151.114	-114.471	23.849
1049	20.188	50.206	36.382	14.501	-152.251	-114.471	23.849
1100	20.280	51.166	37.045	15.533	-152.120	-112.638	22.379
1200	20.450	52.938	38.297	17.569	-151.856	-109.060	19.862
1300	20.620	54.581	39.486	19.623	-151.581	-105.505	17.737
1400	20.800	56.116	40.620	21.694	-151.296	-101.970	15.918
1408	20.814	56.235	40.709	21.860	-151.273	-101.688	15.784
1408	20.814	56.235	40.709	21.860	-153.458	-101.688	15.784
1500	20.970	57.557	41.702	23.782	-153.414	-98.308	14.323
1600	21.140	58.916	42.736	25.888	-153.355	-94.637	12.927
1700	21.320	60.203	43.726	28.011	-153.287	-90.970	11.695
1800	21.500	61.426	44.675	30.152	-153.206	-87.304	10.600
1900	21.680	62.593	45.587	32.311	-153.114	-83.644	9.621

*Enthalpy of formation at 298 K and data above 298 K estimated.

Phase changes: 942 K, α - β transition point of U; $\Delta\text{H}^\circ = 0.667$ kcal/mol.
 1049 K, β - γ transition point of U; $\Delta\text{H}^\circ = 1.137$ kcal/mol.
 1408 K, melting point of U; $\Delta\text{H}^\circ = 2.185$ kcal/mol.

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

298.15-1900 K: $\text{Cp}^\circ = 18.652 + 1.586 \times 10^{-3}\text{T} - 1.284 \times 10^{-5}\text{T}^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 18.652 \times 10^{-3}\text{T} + 0.793 \times 10^{-6}\text{T}^2 + 1.284 \times 10^{-2}\text{T}^{-1} - 6.062$

Reaction equations (kcal/mol):

298.15-942 K: $\Delta\text{Hr}^\circ = -154.620 + 7.616 \times 10^{-3}\text{T} - 3.733 \times 10^{-6}\text{T}^2 + 151.015\text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -154.620 - 7.616 \times 10^{-3}\text{T} \ln \text{T} + 3.733 \times 10^{-6}\text{T}^2 + 75.507\text{T}^{-1} + 87.204 \times 10^{-3}\text{T}$
 942-1049 K: $\Delta\text{Hr}^\circ = -152.210 + 0.471 \times 10^{-3}\text{T} + 0.489 \times 10^{-6}\text{T}^2 + 63.515\text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -152.210 - 0.471 \times 10^{-3}\text{T} \ln \text{T} - 0.489 \times 10^{-6}\text{T}^2 + 31.757\text{T}^{-1} + 39.743 \times 10^{-3}\text{T}$
 1049-1408 K: $\Delta\text{Hr}^\circ = -154.506 + 1.576 \times 10^{-3}\text{T} + 0.489 \times 10^{-6}\text{T}^2 + 63.515\text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -154.506 - 1.576 \times 10^{-3}\text{T} \ln \text{T} - 0.489 \times 10^{-6}\text{T}^2 + 31.757\text{T}^{-1} + 49.618 \times 10^{-3}\text{T}$
 1408-1900 K: $\Delta\text{Hr}^\circ = -153.199 - 0.904 \times 10^{-3}\text{T} + 0.489 \times 10^{-6}\text{T}^2 + 63.515\text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -153.199 + 0.904 \times 10^{-3}\text{T} \ln \text{T} - 0.489 \times 10^{-6}\text{T}^2 + 31.757\text{T}^{-1} + 30.710 \times 10^{-3}\text{T}$

Source: Data from Gronvold (47) who estimated enthalpy of formation at 298 K and data above 298 K.

US₂(β)
β-Uranium Sulfide
[Formation: U(c) + 2S(c,l) = US₂(β)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	17.840	26.390	26.390	0	-124.500	-124.222	91.056
300*	17.860	26.500	26.390	.033	-124.499	-124.220	90.493
368.3	18.297	30.213	26.765	1.270	-124.494	-124.159	73.675
368.3	18.297	30.213	26.765	1.270	-124.686	-124.159	73.675
388.36	18.426	31.187	26.969	1.638	-124.696	-124.129	69.853
388.36	18.426	31.187	26.969	1.638	-125.522	-124.129	69.853
400	18.500	31.732	27.100	1.853	-125.565	-124.087	67.797
432.02	18.625	33.161	27.497	2.447	-125.727	-123.964	62.710
500	18.890	35.904	28.458	3.723	-126.305	-123.635	54.040
600	19.180	39.374	29.996	5.627	-126.912	-123.041	44.817
700	19.430	42.350	31.553	7.558	-127.449	-122.352	38.200
717.824	19.471	42.839	31.827	7.905	-127.540	-122.220	37.211

*Data above 298 K estimated.

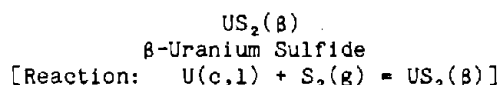
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1800 K: Cp° = 18.233 + 1.984x10⁻³T - 0.876x10⁻⁵T²
H°- H₂₉₈° = 18.233x10⁻³T + 0.992x10⁻⁶T² + 0.876x10⁻²T⁻¹ - 5.818

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -123.696 - 1.225x10⁻³T + 0.204x10⁻⁶T² - 136.100T⁻¹
ΔGf° = -123.696 + 1.225x10⁻³T ln T - 0.204x10⁻⁶T² - 68.050T⁻¹ - 7.916x10⁻³T
368.3-388.36 K: ΔHf° = -125.927 + 3.301x10⁻³T - 3.288x10⁻⁶T² + 175.100T⁻¹
ΔGf° = -125.927 - 3.301x10⁻³T ln T + 3.288x10⁻⁶T² + 87.550T⁻¹ + 22.449x10⁻³T
388.36-432.02 K: ΔHf° = -158.243 + 92.781x10⁻³T - 89.852x10⁻⁶T² + 3979.500T⁻¹
ΔGf° = -158.243 - 92.781x10⁻³T ln T + 89.852x10⁻⁶T² + 1989.750T⁻¹ + 592.906x10⁻³T
432.02-717.824 K: ΔHf° = -177.201 + 84.969x10⁻³T - 50.228x10⁻⁶T² + 10432.500T⁻¹
ΔGf° = -177.201 - 84.969x10⁻³T ln T + 50.228x10⁻⁶T² + 5216.250T⁻¹ + 589.211x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	17.840	26.390	26.390	0	-155.210	-143.249	105.003
300*	17.860	26.500	26.390	.033	-155.203	-143.174	104.301
400	18.500	31.732	27.100	1.853	-154.867	-139.218	76.064
500	18.890	35.904	28.458	3.723	-154.560	-135.341	59.157
600	19.180	39.374	29.996	5.627	-154.301	-131.523	47.907
700	19.430	42.350	31.553	7.558	-154.099	-127.743	39.883
800	19.660	44.960	33.069	9.513	-153.968	-123.987	33.871
900	19.880	47.288	34.521	11.490	-153.920	-120.244	29.199
942	19.972	48.197	35.111	12.327	-153.928	-118.673	27.532
942	19.972	48.197	35.111	12.327	-154.595	-118.673	27.532
1000	20.100	49.394	35.905	13.489	-154.543	-116.462	25.452
1049	20.203	50.358	36.558	14.476	-154.495	-114.596	23.875
1049	20.203	50.358	36.558	14.476	-155.632	-114.596	23.875
1100	20.310	51.319	37.220	15.509	-155.524	-112.604	22.372
1200	20.540	53.096	38.469	17.552	-155.298	-108.712	19.799
1300	20.760	54.749	39.660	19.616	-155.058	-104.842	17.625
1400	20.990	56.296	40.793	21.704	-154.802	-100.986	15.764
1408	21.009	56.416	40.882	21.872	-154.781	-100.679	15.627
1408	21.009	56.416	40.882	21.872	-156.966	-100.679	15.627
1500	21.230	57.752	41.875	23.815	-156.943	-97.001	14.133
1600	21.480	59.130	42.911	25.950	-156.902	-93.008	12.704
1700	21.730	60.440	43.904	28.111	-156.843	-89.016	11.444
1800	22.000	61.690	44.858	30.297	-156.764	-85.029	10.324

*Data above 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.

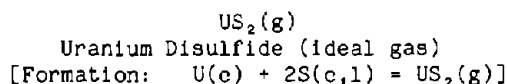
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

$$298.15-1800 \text{ K: } \begin{aligned} \text{Cp}^\circ &= 18.233 + 1.984 \times 10^{-3}T - 0.876 \times 10^{-5}T^2 \\ \text{H}^\circ - \text{H}_{298}^\circ &= 18.233 \times 10^{-3}T + 0.992 \times 10^{-6}T^2 + 0.876 \times 10^{-2}T^{-1} - 5.818 \end{aligned}$$

Reaction equations (kcal/mol):

$$\begin{aligned} 298.15-942 \text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= -157.274 + 6.780 \times 10^{-3}T - 3.550 \times 10^{-6}T^2 + 106.800T^{-1} \\ \Delta \text{Gr}^\circ &= -157.274 - 6.780 \times 10^{-3}T \ln T + 3.550 \times 10^{-6}T^2 + 53.400T^{-1} + 84.010 \times 10^{-3}T \end{aligned} \\ 942-1049 \text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= -154.864 - 0.365 \times 10^{-3}T + 0.672 \times 10^{-6}T^2 + 19.300T^{-1} \\ \Delta \text{Gr}^\circ &= -154.864 + 0.365 \times 10^{-3}T \ln T - 0.672 \times 10^{-6}T^2 + 9.650T^{-1} + 36.549 \times 10^{-3}T \end{aligned} \\ 1049-1408 \text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= -157.160 + 0.740 \times 10^{-3}T + 0.672 \times 10^{-6}T^2 + 19.300T^{-1} \\ \Delta \text{Gr}^\circ &= -157.160 - 0.740 \times 10^{-3}T \ln T - 0.672 \times 10^{-6}T^2 + 9.650T^{-1} + 46.423 \times 10^{-3}T \end{aligned} \\ 1408-1800 \text{ K: } \begin{aligned} \Delta \text{Hr}^\circ &= -155.853 - 1.740 \times 10^{-3}T + 0.672 \times 10^{-6}T^2 + 19.300T^{-1} \\ \Delta \text{Gr}^\circ &= -155.853 + 1.740 \times 10^{-3}T \ln T - 0.672 \times 10^{-6}T^2 + 9.650T^{-1} + 27.515 \times 10^{-3}T \end{aligned} \end{aligned}$$

Sources: Enthalpy of formation at 298 K from Settle (106). Other data are from Gronvold (47) who estimated all above 298 K.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHf°	ΔGf°	
298.15*	13.756	68.630	68.630	0	21.400	9.084	-6.659
300	13.768	68.715	68.632	.025	21.393	9.008	-6.562
368.3	14.075	71.575	68.918	.979	21.115	6.216	-3.689
368.3	14.075	71.575	68.918	.979	20.923	6.216	-3.689
388.36	14.166	72.324	69.075	1.262	20.828	5.419	-3.049
388.36	14.166	72.324	69.075	1.262	20.002	5.419	-3.049
400	14.218	72.743	69.175	1.427	19.909	4.983	-2.722
432.02	14.292	73.841	69.481	1.883	19.609	3.798	-1.921
500	14.450	75.942	70.220	2.861	18.733	1.384	-.605
600	14.583	78.589	71.401	4.313	17.674	-1.984	.723
700	14.665	80.844	72.593	5.776	16.669	-5.180	1.617
717.824	14.675	81.213	72.802	6.037	16.493	-5.733	1.745

*Data except enthalpy of formation at 298 K estimated.

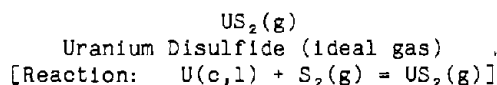
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta\text{H}^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta\text{H}^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta\text{H}^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $\text{Cp}^\circ = 14.800 + 0.066 \times 10^{-3}T - 0.946 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 14.800 \times 10^{-3}T + 0.033 \times 10^{-6}T^2 + 0.946 \times 10^{-2}T^3 - 4.733$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta\text{Hf}^\circ = 23.289 - 4.658 \times 10^{-3}T - 0.755 \times 10^{-6}T^2 - 129.100T^{-1}$
 $\Delta\text{Gf}^\circ = 23.289 + 4.658 \times 10^{-3}T \ln T + 0.755 \times 10^{-6}T^2 - 64.550T^{-1} - 73.682 \times 10^{-3}T$
 368.3-388.36 K: $\Delta\text{Hf}^\circ = 21.059 - 0.132 \times 10^{-3}T - 4.247 \times 10^{-6}T^2 + 182.100T^{-1}$
 $\Delta\text{Gf}^\circ = 21.059 + 0.132 \times 10^{-3}T \ln T + 4.247 \times 10^{-6}T^2 + 91.050T^{-1} - 43.316 \times 10^{-3}T$
 388.36-432.02 K: $\Delta\text{Hf}^\circ = -11.258 + 89.348 \times 10^{-3}T - 90.811 \times 10^{-6}T^2 + 3986.500T^{-1}$
 $\Delta\text{Gf}^\circ = -11.258 - 89.348 \times 10^{-3}T \ln T + 90.811 \times 10^{-6}T^2 + 1993.250T^{-1} + 527.141 \times 10^{-3}T$
 432.02-717.824 K: $\Delta\text{Hf}^\circ = -30.215 + 81.536 \times 10^{-3}T - 51.187 \times 10^{-6}T^2 + 10439.500T^{-1}$
 $\Delta\text{Gf}^\circ = -30.215 - 81.536 \times 10^{-3}T \ln T + 51.187 \times 10^{-6}T^2 + 5219.750T^{-1} + 523.446 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHr°	ΔGr°	
298.15*	13.756	68.630	68.630	0	-9.310	-9.943	7.289
300	13.768	68.715	68.632	.025	-9.311	-9.947	7.246
400	14.218	72.743	69.175	1.427	-9.393	-10.149	5.545
500	14.450	75.942	70.220	2.861	-9.522	-10.323	4.512
600	14.583	78.589	71.401	4.313	-9.715	-10.466	3.812
700	14.665	80.844	72.593	5.776	-9.981	-10.570	3.300
800	14.720	82.806	73.750	7.245	-10.336	-10.632	2.904
900	14.758	84.542	74.854	8.719	-10.791	-10.643	2.585
942	14.769	85.215	75.301	9.339	-11.016	-10.632	2.467
942	14.769	85.215	75.301	9.339	-11.683	-10.632	2.467
1000	14.785	86.098	75.902	10.196	-11.936	-10.559	2.308
1049	14.795	86.806	76.395	10.921	-12.151	-10.485	2.184
1049	14.795	86.806	76.395	10.921	-13.288	-10.485	2.184
1100	14.805	87.508	76.893	11.676	-13.457	-10.345	2.055
1200	14.821	88.797	77.833	13.157	-13.793	-10.048	1.830
1300	14.833	89.984	78.722	14.640	-14.134	-9.723	1.635
1400	14.843	91.084	79.568	16.123	-14.483	-9.370	1.463
1408	14.844	91.169	79.633	16.242	-14.511	-9.341	1.450
1408	14.844	91.169	79.633	16.242	-16.696	-9.341	1.450
1500	14.851	92.108	80.369	17.608	-17.250	-8.843	1.288
1600	14.857	93.067	81.133	19.094	-17.858	-8.263	1.129
1700	14.862	93.968	81.862	20.580	-18.474	-7.645	.983
1800	14.867	94.817	82.558	22.066	-19.095	-6.988	.848
1900	14.871	95.621	83.225	23.553	-19.722	-6.299	.724
2000	14.874	96.384	83.864	25.040	-20.355	-5.577	.609

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 942 K, $\alpha - \beta$ transition point of U; $\Delta \text{H}^\circ = 0.667$ kcal/mol.
 1049 K, $\beta - \gamma$ transition point of U; $\Delta \text{H}^\circ = 1.137$ kcal/mol.
 1408 K, melting point of U; $\Delta \text{H}^\circ = 2.185$ kcal/mol.

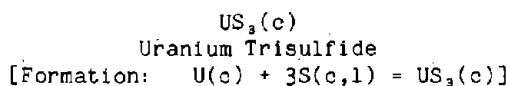
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-2000 K: $\text{Cp}^\circ = 14.800 + 0.066 \times 10^{-3} \text{T} - 0.946 \times 10^{-5} \text{T}^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 14.800 \times 10^{-3} \text{T} + 0.033 \times 10^{-6} \text{T}^2 + 0.946 \times 10^{-2} \text{T}^{-1} - 4.733$

Reaction equations (kcal/mol):

298.15-942 K: $\Delta \text{Hr}^\circ = -10.289 + 3.347 \times 10^{-3} \text{T} - 4.509 \times 10^{-6} \text{T}^2 + 113.800 \text{T}^{-1}$
 $\Delta \text{Gr}^\circ = -10.289 - 3.347 \times 10^{-3} \text{T} \ln \text{T} + 4.509 \times 10^{-6} \text{T}^2 + 56.900 \text{T}^{-1} + 18.244 \times 10^{-3} \text{T}$
 942-1049 K: $\Delta \text{Hr}^\circ = -7.879 - 3.798 \times 10^{-3} \text{T} - 0.287 \times 10^{-6} \text{T}^2 + 26.300 \text{T}^{-1}$
 $\Delta \text{Gr}^\circ = -7.879 + 3.798 \times 10^{-3} \text{T} \ln \text{T} + 0.287 \times 10^{-6} \text{T}^2 + 13.150 \text{T}^{-1} - 29.217 \times 10^{-3} \text{T}$
 1049-1408 K: $\Delta \text{Hr}^\circ = -10.175 - 2.693 \times 10^{-3} \text{T} - 0.287 \times 10^{-6} \text{T}^2 + 26.300 \text{T}^{-1}$
 $\Delta \text{Gr}^\circ = -10.175 + 2.693 \times 10^{-3} \text{T} \ln \text{T} + 0.287 \times 10^{-6} \text{T}^2 + 13.150 \text{T}^{-1} - 19.342 \times 10^{-3} \text{T}$
 1408-2000 K: $\Delta \text{Hr}^\circ = -8.868 - 5.173 \times 10^{-3} \text{T} - 0.287 \times 10^{-6} \text{T}^2 + 26.300 \text{T}^{-1}$
 $\Delta \text{Gr}^\circ = -8.868 + 5.173 \times 10^{-3} \text{T} \ln \text{T} + 0.287 \times 10^{-6} \text{T}^2 + 13.150 \text{T}^{-1} - 38.250 \times 10^{-3} \text{T}$

Source: Data from Gronvold (47) who estimated all except enthalpy of formation at 298 K.



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHf°	ΔGf°	
298.15	22.850	33.100	33.100	0	-130.100	-129.539	94.953
300*	22.880	33.241	33.101	.042	-130.100	-129.535	94.365
368.3	23.652	38.021	33.581	1.636	-130.122	-129.405	76.788
368.3	23.652	38.021	33.581	1.636	-130.410	-129.405	76.788
388.36	23.878	39.282	33.843	2.112	-130.430	-129.348	72.790
388.36	23.878	39.282	33.843	2.112	-131.669	-129.348	72.790
400	24.010	39.989	34.011	2.391	-131.737	-129.278	70.633
432.02	24.225	41.846	34.524	3.163	-131.984	-129.074	65.295
500	24.680	45.422	35.768	4.827	-132.848	-128.539	56.183
600	25.170	49.967	37.767	7.320	-133.723	-127.591	46.474
700	25.570	53.877	39.796	9.857	-134.454	-126.509	39.497
717.824	25.634	54.521	40.153	10.313	-134.572	-126.304	38.454

*Data above 298 K estimated.

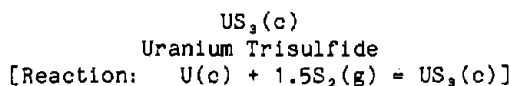
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta\text{H}^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta\text{H}^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta\text{H}^\circ = 0$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-1100 K: $\text{Cp}^\circ = 23.986 + 2.760 \times 10^{-3}\text{T} - 1.741 \times 10^{-5}\text{T}^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 23.986 \times 10^{-3}\text{T} + 1.380 \times 10^{-6}\text{T}^2 + 1.741 \times 10^{-2}\text{T}^{-1} - 7.858$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta\text{Hf}^\circ = -128.530 - 3.646 \times 10^{-3}\text{T} + 2.309 \times 10^{-6}\text{T}^2 - 205.200\text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -128.530 + 3.646 \times 10^{-3}\text{T} \ln \text{T} - 2.309 \times 10^{-6}\text{T}^2 - 102.600\text{T}^{-1} - 22.314 \times 10^{-3}\text{T}$
 368.3-388.36 K: $\Delta\text{Hf}^\circ = -131.875 + 3.143 \times 10^{-3}\text{T} - 2.929 \times 10^{-6}\text{T}^2 + 261.600\text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -131.875 - 3.143 \times 10^{-3}\text{T} \ln \text{T} + 2.929 \times 10^{-6}\text{T}^2 + 130.800\text{T}^{-1} + 23.235 \times 10^{-3}\text{T}$
 388.36-432.02 K: $\Delta\text{Hf}^\circ = -180.350 + 137.363 \times 10^{-3}\text{T} - 132.775 \times 10^{-6}\text{T}^2 + 5968.200\text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -180.350 - 137.363 \times 10^{-3}\text{T} \ln \text{T} + 132.775 \times 10^{-6}\text{T}^2 + 2984.100\text{T}^{-1} + 878.920 \times 10^{-3}\text{T}$
 432.02-717.824 K: $\Delta\text{Hf}^\circ = -208.786 + 125.645 \times 10^{-3}\text{T} - 73.339 \times 10^{-6}\text{T}^2 + 15647.700\text{T}^{-1}$
 $\Delta\text{Gf}^\circ = -208.786 - 125.645 \times 10^{-3}\text{T} \ln \text{T} + 73.339 \times 10^{-6}\text{T}^2 + 7823.850\text{T}^{-1} + 873.378 \times 10^{-3}\text{T}$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	$-(\text{G}^\circ - \text{H}_{298}^\circ)/\text{T}$	$\text{H}^\circ - \text{H}_{298}^\circ$	ΔHr°	ΔGr°	
298.15	22.850	33.100	33.100	0	-176.165	-158.080	115.874
300*	22.880	33.241	33.101	.042	-176.156	-157.966	115.077
400	24.010	39.989	34.011	2.391	-175.690	-151.975	83.034
500	24.680	45.422	35.768	4.827	-175.230	-146.098	63.859
600	25.170	49.967	37.767	7.320	-174.807	-140.314	51.109
700	25.570	53.877	39.796	9.857	-174.429	-134.594	42.022
800	25.930	57.316	41.775	12.433	-174.113	-128.926	35.220
900	26.250	60.388	43.675	15.042	-173.873	-123.293	29.939
942	26.380	61.588	44.447	16.147	-173.798	-120.935	28.057
942	26.380	61.588	44.447	16.147	-174.465	-120.935	28.057
1000	26.560	63.170	45.488	17.682	-174.298	-117.645	25.711
1049	26.707	64.444	46.344	18.987	-174.151	-114.871	23.932
1049	26.707	64.444	46.344	18.987	-175.288	-114.871	23.932
1100	26.860	65.716	47.213	20.353	-175.076	-111.940	22.240

*Data above 298 K estimated.

Phase changes: 942 K, $\alpha - \beta$ transition point of U; $\Delta\text{H}^\circ = 0.667$ kcal/mol.
 1049 K, $\beta - \gamma$ transition point of U; $\Delta\text{H}^\circ = 1.137$ kcal/mol.

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

298.15-1100 K: $\text{Cp}^\circ = 23.986 + 2.760 \times 10^{-3}\text{T} - 1.741 \times 10^{-5}\text{T}^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 23.986 \times 10^{-3}\text{T} + 1.380 \times 10^{-6}\text{T}^2 + 1.741 \times 10^{-2}\text{T}^{-1} - 7.858$

Reaction equations (kcal/mol):

298.15-942 K: $\Delta\text{Hr}^\circ = -178.896 + 8.361 \times 10^{-3}\text{T} - 3.322 \times 10^{-5}\text{T}^2 + 159.150\text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -178.896 - 8.361 \times 10^{-3}\text{T} \ln \text{T} + 3.322 \times 10^{-6}\text{T}^2 + 79.575\text{T}^{-1} + 115.575 \times 10^{-3}\text{T}$
 942-1049 K: $\Delta\text{Hr}^\circ = -176.486 + 1.216 \times 10^{-3}\text{T} + 0.900 \times 10^{-6}\text{T}^2 + 71.650\text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -176.486 - 1.216 \times 10^{-3}\text{T} \ln \text{T} - 0.900 \times 10^{-6}\text{T}^2 + 35.825\text{T}^{-1} + 68.114 \times 10^{-3}\text{T}$
 1049-1100 K: $\Delta\text{Hr}^\circ = -178.783 + 2.322 \times 10^{-3}\text{T} + 0.900 \times 10^{-6}\text{T}^2 + 71.650\text{T}^{-1}$
 $\Delta\text{Gr}^\circ = -178.783 - 2.322 \times 10^{-3}\text{T} \ln \text{T} - 0.900 \times 10^{-6}\text{T}^2 + 35.825\text{T}^{-1} + 77.989 \times 10^{-3}\text{T}$

Source: Data from Gronvold (47) who estimated all above 298 K.

$V_2S_3(c)$
Divanadium Trisulfide
[Formation: $2V(c) + 3S(c,l) = V_2S_3(c)$]

T, K	cal/mol·K			kcal/mol			Log Kf
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15*	22.200	30.500	30.500	0	-125.000	-123.118	90.247
300	22.310	30.640	30.503	1.041	-125.011	-123.106	89.682
368.3	25.220	35.562	30.987	1.685	-125.350	-122.634	72.770
368.3	25.220	35.562	30.987	1.685	-125.638	-122.634	72.770
388.36	26.074	36.923	31.259	2.200	-125.730	-122.466	68.917
388.36	26.074	36.923	31.259	2.200	-126.969	-122.466	68.917
400	26.570	37.700	31.435	2.506	-127.072	-122.331	66.838
432.02	27.431	39.779	31.977	3.371	-127.400	-121.940	61.686
500	29.260	43.930	33.320	5.305	-128.356	-120.995	52.886
600	31.320	49.460	35.565	8.337	-129.195	-119.439	43.505
700	33.090	54.420	37.906	11.560	-129.700	-117.768	36.768
717.824	33.379	55.255	38.326	12.152	-129.758	-117.462	35.762

*Enthalpy of formation and entropy at 298 K estimated.

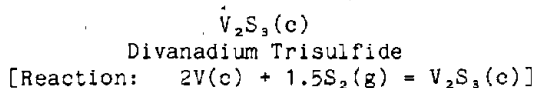
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-1200 K: $C_p^\circ = 25.049 + 13.254 \times 10^{-3}T - 6.047 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 25.049 \times 10^{-3}T + 6.627 \times 10^{-6}T^2 + 6.047 \times 10^{-2}T^{-1} - 10.086$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -123.527 - 9.695 \times 10^{-3}T + 9.554 \times 10^{-6}T^2 + 169.300T^{-1}$
 $\Delta G_f^\circ = -123.527 + 9.695 \times 10^{-3}T \ln T - 9.554 \times 10^{-6}T^2 + 84.650T^{-1} + 51.971 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = -126.872 - 2.906 \times 10^{-3}T + 4.316 \times 10^{-6}T^2 + 636.100T^{-1}$
 $\Delta G_f^\circ = -126.872 + 2.906 \times 10^{-3}T \ln T - 4.316 \times 10^{-6}T^2 + 318.050T^{-1} - 6.422 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = -175.347 + 131.314 \times 10^{-3}T - 125.530 \times 10^{-6}T^2 + 6342.700T^{-1}$
 $\Delta G_f^\circ = -175.347 - 131.314 \times 10^{-3}T \ln T + 125.530 \times 10^{-6}T^2 + 3171.350T^{-1} + 849.263 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = -203.783 + 119.596 \times 10^{-3}T - 66.094 \times 10^{-6}T^2 + 16022.200T^{-1}$
 $\Delta G_f^\circ = -203.783 - 119.596 \times 10^{-3}T \ln T + 66.094 \times 10^{-6}T^2 + 8011.100T^{-1} + 843.721 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15*	22.200	30.500	30.500	0	-171.065	-151.659	111.167
300	22.310	30.640	30.503	.041	-171.067	-151.538	110.394
400	26.570	37.700	31.435	2.506	-171.025	-145.028	79.238
500	29.260	43.930	33.320	5.305	-170.738	-138.554	60.561
600	31.320	49.460	35.565	8.337	-170.279	-132.162	48.139
700	33.090	54.420	37.906	11.560	-169.675	-125.853	39.293
800	34.710	58.950	40.261	14.951	-168.945	-119.643	32.685
900	36.230	63.120	42.567	18.498	-168.104	-113.525	27.567
1000	37.700	67.020	44.825	22.195	-167.159	-107.517	23.498
1100	39.130	70.680	47.010	26.037	-166.116	-101.602	20.186
1200	40.530	74.140	49.123	30.020	-164.984	-95.779	17.443

*Enthalpy of formation and entropy at 298 K estimated.

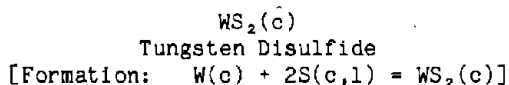
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1200 K: $C_p^\circ = 25.049 + 13.254 \times 10^{-3}T - 6.047 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 25.049 \times 10^{-3}T + 6.627 \times 10^{-6}T^2 + 6.047 \times 10^{-2}T^{-1} - 10.086$

Reaction equations (kcal/mol):

298.15-1200 K: $\Delta H_r^\circ = -173.893 + 2.312 \times 10^{-3}T + 3.923 \times 10^{-6}T^2 + 533.650T^{-1}$
 $\Delta G_r^\circ = -173.893 - 2.312 \times 10^{-3}T \ln T - 3.923 \times 10^{-6}T^2 + 266.825T^{-1} + 85.918 \times 10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K are those estimated by Mills (80). Other data based on Bolgar (12).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	15.253	16.200	16.200	0	-57.550	-55.486	40.672
300	15.289	16.295	16.200	.029	-57.552	-55.471	40.410
368.3	16.218	19.549	16.524	1.114	-57.637	-54.989	32.630
368.3	16.218	19.549	16.524	1.114	-57.829	-54.989	32.630
388.36	16.491	20.417	16.703	1.442	-57.858	-54.832	30.856
388.36	16.491	20.417	16.703	1.442	-58.684	-54.832	30.856
400	16.649	20.906	16.819	1.635	-58.737	-54.716	29.895
432.02	16.859	22.196	17.170	2.171	-58.919	-54.389	27.514
500	17.304	24.699	18.025	3.337	-59.515	-53.623	23.438
600	17.686	27.892	19.415	5.086	-60.098	-52.393	19.084
700	17.945	30.638	20.825	6.869	-60.541	-51.067	15.944
717.824	17.979	31.090	21.074	7.189	-60.607	-50.824	15.474

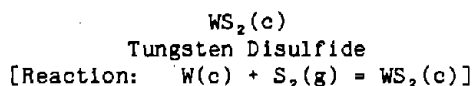
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
 388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
 432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1500 K: Cp° = 17.917 + 0.806x10⁻³T - 2.582x10⁻⁵T²
 H° - H°₂₉₈ = 17.917x10⁻³T + 0.403x10⁻⁶T² + 2.582x10⁻²T⁻¹ - 6.244

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = -56.344 - 4.246x10⁻³T + 3.466x10⁻⁶T² - 74.000T⁻¹
 ΔGf° = -56.344 + 4.246x10⁻³T lnT - 3.466x10⁻⁶T² - 37.000T⁻¹ - 19.865x10⁻³T
 368.3-388.36 K: ΔHf° = -58.574 + 0.280x10⁻³T - 0.026x10⁻⁶T² + 237.200T⁻¹
 ΔGf° = -58.574 - 0.280x10⁻³T lnT + 0.026x10⁻⁶T² + 118.600T⁻¹ + 10.500x10⁻³T
 388.36-432.02 K: ΔHf° = -90.891 + 89.760x10⁻³T - 86.590x10⁻⁶T² + 4041.600T⁻¹
 ΔGf° = -90.891 - 89.760x10⁻³T lnT + 86.590x10⁻⁶T² + 2020.800T⁻¹ + 580.957x10⁻³T
 432.02-717.824 K: ΔHf° = -109.848 + 81.948x10⁻³T - 46.966x10⁻⁶T² + 10494.600T⁻¹
 ΔGf° = -109.848 - 81.948x10⁻³T lnT + 46.966x10⁻⁶T² + 5247.300T⁻¹ + 577.262x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	15.253	16.200	16.200	0	-88.260	-74.513	54.619
300	15.289	16.295	16.200	.029	-88.256	-74.426	54.219
400	16.649	20.906	16.819	1.635	-88.039	-69.847	38.162
500	17.304	24.699	18.025	3.337	-87.770	-65.329	28.555
600	17.686	27.892	19.415	5.086	-87.487	-60.875	22.173
700	17.945	30.638	20.825	6.869	-87.191	-56.458	17.627
800	18.138	33.047	22.205	8.674	-86.889	-52.089	14.230
900	18.298	35.194	23.533	10.495	-86.589	-47.756	11.597
1000	18.439	37.130	24.797	12.333	-86.283	-43.456	9.497
1100	18.571	38.893	25.999	14.183	-85.981	-39.179	7.784
1200	18.697	40.514	27.142	16.047	-85.681	-34.944	6.364
1300	18.822	42.015	28.228	17.923	-85.383	-30.722	5.165
1400	18.948	43.415	29.264	19.811	-85.091	-26.519	4.140
1500	19.077	44.725	30.251	21.711	-84.801	-22.350	3.256

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

298.15-1500 K: $C_p^\circ = 17.917 + 0.806 \times 10^{-3}T - 2.582 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 17.917 \times 10^{-3}T + 0.403 \times 10^{-6}T^2 + 2.582 \times 10^{-2}T^{-1} - 6.244$

Reaction equations (kcal/mol):

298.15-1500 K: $\Delta H_r^\circ = -89.922 + 3.759 \times 10^{-3}T - 0.288 \times 10^{-6}T^2 + 168.900T^{-1}$
 $\Delta G_r^\circ = -89.922 - 3.759 \times 10^{-3}T \ln T + 0.288 \times 10^{-6}T^2 + 84.450T^{-1} + 72.061 \times 10^{-3}T$

Source: Data from O'Hare (88).

YS(g)
Yttrium Monosulfide (ideal gas)
[Formation: Y(c) + S(c,l) = YS(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	8.160	58.530	58.530	0	41.200	29.200	-21.404
300	8.170	58.580	58.530	.015	41.193	29.126	-21.218
368.3	8.382	60.284	58.702	.583	40.941	26.403	-15.667
368.3	8.382	60.284	58.702	.583	40.845	26.403	-15.667
388.36	8.444	60.730	58.795	.752	40.765	25.619	-14.417
388.36	8.444	60.730	58.795	.752	40.352	25.619	-14.417
400	8.480	60.980	58.855	.850	40.287	25.179	-13.757
432.02	8.528	61.635	59.037	1.122	40.088	23.976	-12.129
500	8.630	62.890	59.478	1.706	39.549	21.488	-9.392
600	8.710	64.470	60.182	2.573	38.886	17.941	-6.535
700	8.760	65.820	60.896	3.447	38.269	14.494	-4.525
717.824	8.767	66.040	61.021	3.603	38.163	13.891	-4.229

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 8.866 + 0.040x10⁻⁵T - 0.640x10⁻⁹T²
H° - H°₂₉₈ = 8.866x10⁻³T + 0.020x10⁻⁶T² + 0.640x10⁻²T³ - 2.860

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 42.907 - 5.026x10⁻³T + 0.832x10⁻⁶T² - 84.300T⁻¹
ΔGf° = 42.907 + 5.026x10⁻³T lnT - 0.832x10⁻⁶T² - 42.150T⁻¹ - 73.889x10⁻³T
368.3-388.36 K: ΔHf° = 41.792 - 2.763x10⁻³T - 0.914x10⁻⁶T² + 71.300T⁻¹
ΔGf° = 41.792 + 2.763x10⁻³T lnT + 0.914x10⁻⁶T² + 35.650T⁻¹ - 58.706x10⁻³T
388.36-432.02 K: ΔHf° = 25.634 + 41.977x10⁻³T - 44.196x10⁻⁶T² + 1973.500T⁻¹
ΔGf° = 25.634 - 41.977x10⁻³T lnT + 44.196x10⁻⁶T² + 986.750T⁻¹ + 226.522x10⁻³T
432.02-717.824 K: ΔHf° = 16.155 + 38.071x10⁻³T - 24.384x10⁻⁶T² + 5200.000T⁻¹
ΔGf° = 16.155 - 38.071x10⁻³T lnT + 24.384x10⁻⁶T² + 2600.000T⁻¹ + 224.675x10⁻³T

YS(g)
Yttrium Monosulfide (ideal gas)
[Reaction: $\text{Y(c,l)} + 0.5\text{S}_2(\text{g}) = \text{YS(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15*	8.160	58.530	58.530	0	25.845	19.686	-14.430
300	8.170	58.580	58.530	.015	25.841	19.648	-14.314
400	8.480	60.980	58.855	.850	25.636	17.613	-9.623
500	8.630	62.890	59.478	1.706	25.422	15.634	-6.834
600	8.710	64.470	60.182	2.573	25.192	13.700	-4.990
700	8.760	65.820	60.896	3.447	24.944	11.799	-3.684
800	8.800	66.990	61.582	4.326	24.679	9.945	-2.717
900	8.820	68.030	62.244	5.207	24.393	8.112	-1.970
1000	8.840	68.960	62.870	6.090	24.087	6.326	-1.382
1100	8.860	69.800	63.459	6.975	23.762	4.562	-.906
1200	8.870	70.570	64.019	7.861	23.417	2.833	-.516
1300	8.880	71.280	64.550	8.749	23.052	1.135	-.191
1400	8.890	71.940	65.056	9.637	22.666	-.531	.083
1500	8.900	72.560	65.542	10.527	22.259	-2.192	.319
1600	8.900	73.130	65.994	11.417	21.831	-3.801	.519
1700	8.910	73.670	66.430	12.308	21.383	-5.384	.692
1752	8.915	73.939	66.650	12.771	21.139	-6.197	.773
1752	8.915	73.939	66.650	12.771	19.946	-6.197	.773
1799	8.920	74.175	66.843	13.190	19.749	-6.904	.839
1799	8.920	74.175	66.843	13.190	17.025	-6.904	.839
1800	8.920	74.180	66.847	13.199	17.020	-6.912	.839
1900	8.920	74.660	67.244	14.091	16.406	-8.215	.945
2000	8.930	75.120	67.628	14.984	15.791	-9.515	1.040

*Data except enthalpy of formation at 298 K estimated.

Phase changes: 1752 K, $\alpha - \beta$ transition point of Y; $\Delta H^\circ = 1.193$ kcal/mol.
1799 K, melting point of Y; $\Delta H^\circ = 2.274$ kcal/mol.

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

298.15-2000 K: $C_p^\circ = 8.866 + 0.040 \times 10^{-3}T - 0.640 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 8.866 \times 10^{-3}T + 0.020 \times 10^{-6}T^2 + 0.640 \times 10^{-2}T^{-1} - 2.860$

Reaction equations (kcal/mol):

298.15-1752 K: $\Delta H_r^\circ = 26.118 - 1.024 \times 10^{-3}T - 1.045 \times 10^{-6}T^2 + 37.150T^{-1}$
 $\Delta G_r^\circ = 26.118 + 1.024 \times 10^{-3}T \ln T + 1.045 \times 10^{-6}T^2 + 18.575T^{-1} - 27.926 \times 10^{-3}T$
1752-1799 K: $\Delta H_r^\circ = 26.780 - 3.665 \times 10^{-3}T - 0.140 \times 10^{-6}T^2 + 29.850T^{-1}$
 $\Delta G_r^\circ = 26.780 + 3.665 \times 10^{-3}T \ln T + 0.140 \times 10^{-6}T^2 + 14.925T^{-1} - 46.449 \times 10^{-3}T$
1799-2000 K: $\Delta H_r^\circ = 27.547 - 5.606 \times 10^{-3}T - 0.140 \times 10^{-6}T^2 + 29.850T^{-1}$
 $\Delta G_r^\circ = 27.547 + 5.606 \times 10^{-3}T \ln T + 0.140 \times 10^{-6}T^2 + 14.925T^{-1} - 61.415 \times 10^{-3}T$

Source: Data from Mills (80) who estimated all except enthalpy of formation at 298 K.

YbS(g)
Ytterbium Monosulfide (ideal gas)
[Formation: Yb(c) + S(c,l) = YbS(g)]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15*	8.400	61.490	61.490	0	63.000	51.214	-37.541
300	8.410	61.540	61.490	.016	62.994	51.142	-37.257
368.3	8.560	63.290	61.671	.597	62.752	48.467	-28.760
368.3	8.560	63.290	61.671	.597	62.656	48.467	-28.760
388.36	8.604	63.746	61.766	.769	62.577	47.697	-26.841
388.36	8.604	63.746	61.766	.769	62.164	47.697	-26.841
400	8.630	64.000	61.827	.869	62.100	47.264	-25.823
432.02	8.665	64.666	62.014	1.146	61.898	46.083	-23.312
500	8.740	65.930	62.454	1.738	61.339	43.648	-19.078
553	8.766	66.814	62.831	2.202	60.926	41.793	-16.517
600	8.790	67.530	63.172	2.615	60.609	40.180	-14.635
700	8.830	68.890	63.896	3.496	59.972	36.827	-11.498
717.824	8.834	69.112	64.022	3.653	59.863	36.240	-11.034

*Data except enthalpy of formation at 298 K estimated.

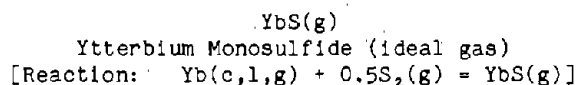
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; ΔH° = 0.096 kcal/mol.
388.36 K, melting point of S; ΔH° = 0.413 kcal/mol.
432.02 K, second order transformation of S; ΔH° = 0 kcal/mol.
553 K, second order transition of Yb; ΔH° = 0 kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-2000 K: Cp° = 8.910 + 0.018x10⁻³T - 0.454x10⁻⁵T⁻²
H° - H₂₉₈° = 8.910x10⁻³T + 0.009x10⁻⁶T² + 0.454x10⁻³T⁻¹ - 2.810

Formation equations (kcal/mol):

298.15-368.3 K: ΔHf° = 63.223 - 0.288x10⁻³T - 3.976x10⁻⁶T² + 64.500T⁻¹
ΔGf° = 63.223 + 0.288x10⁻³T ln T + 3.976x10⁻⁶T² + 32.250T⁻¹ - 43.466x10⁻³T
368.3-388.36 K: ΔHf° = 62.108 + 1.975x10⁻³T - 5.722x10⁻⁶T² + 220.100T⁻¹
ΔGf° = 62.108 - 1.975x10⁻³T ln T + 5.722x10⁻⁶T² + 110.050T⁻¹ - 28.283x10⁻³T
388.36-432.02 K: ΔHf° = 45.950 + 46.715x10⁻³T - 49.004x10⁻⁶T² + 2122.300T⁻¹
ΔGf° = 45.950 - 46.715x10⁻³T ln T + 49.004x10⁻⁶T² + 1061.150T⁻¹ + 256.945x10⁻³T
432.02-553 K: ΔHf° = 36.471 + 42.809x10⁻³T - 29.192x10⁻⁶T² + 5348.800T⁻¹
ΔGf° = 36.471 - 42.809x10⁻³T ln T + 29.192x10⁻⁶T² + 2674.400T⁻¹ + 255.098x10⁻³T
553-717.824 K: ΔHf° = 38.092 + 37.605x10⁻³T - 24.184x10⁻⁶T² + 5196.800T⁻¹
ΔGf° = 38.092 - 37.605x10⁻³T ln T + 24.184x10⁻⁶T² + 2598.400T⁻¹ + 222.319x10⁻³T



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHr°	ΔGr°	
298.15*	8.400	61.490	61.490	0	47.645	41.701	-30.567
300	8.410	61.540	61.490	.016	47.642	41.665	-30.353
400	8.630	64.000	61.827	.869	47.449	39.698	-21.690
500	8.740	65.930	62.454	1.738	47.212	37.794	-16.520
553	8.766	66.814	62.831	2.202	47.036	36.804	-14.545
600	8.790	67.530	63.172	2.615	46.915	35.939	-13.091
700	8.830	68.890	63.896	3.496	46.647	34.132	-10.656
800	8.850	70.070	64.594	4.381	46.365	32.360	-8.840
900	8.870	71.120	65.268	5.267	46.068	30.624	-7.437
1000	8.880	72.050	65.896	6.154	45.755	28.924	-6.321
1033	8.883	72.338	66.097	6.447	45.647	28.372	-6.003
1033	8.883	72.338	66.097	6.447	45.229	28.372	-6.003
1097	8.890	72.876	66.480	7.016	44.958	27.338	-5.446
1097	8.890	72.876	66.480	7.016	43.128	27.338	-5.446
1100	8.890	72.900	66.497	7.043	43.117	27.293	-5.423
1200	8.900	73.670	67.060	7.932	42.675	25.873	-4.712
1300	8.910	74.380	67.593	8.823	42.233	24.502	-4.119
1400	8.910	75.040	68.101	9.714	41.786	23.154	-3.614
1467	8.917	75.462	68.433	10.311	41.485	22.261	-3.316
1467	8.917	75.462	68.433	10.311	10.685	22.261	-3.316
1500	8.920	75.660	68.590	10.605	10.663	22.524	-3.282
1600	8.920	76.230	69.044	11.497	10.592	23.325	-3.186
1700	8.920	76.780	69.492	12.389	10.519	24.109	-3.099
1800	8.930	77.290	69.912	13.281	10.441	24.911	-3.025
1900	8.930	77.770	70.310	14.174	10.362	25.721	-2.959
2000	8.930	78.230	70.697	15.067	10.280	26.528	-2.899

*Data except enthalpy of formation at 298 K estimated.

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:

$$298.15-2000 \text{ K: } \begin{aligned} C_p^\circ &= 8.910 + 0.018 \times 10^{-3} T - 0.454 \times 10^{-5} T^2 \\ H^\circ - H_{298}^\circ &= 8.910 \times 10^{-3} T + 0.009 \times 10^{-6} T^2 + 0.454 \times 10^{-2} T^{-1} - 2.810 \end{aligned}$$

Reaction equations (kcal/mol):

$$\begin{aligned} 298.15-553 \text{ K: } \begin{aligned} \Delta H_r^\circ &= 46.434 + 3.714 \times 10^{-3} T - 5.853 \times 10^{-6} T^2 + 185.950 T^{-1} \\ \Delta G_r^\circ &= 46.434 - 3.714 \times 10^{-3} T \ln T + 5.853 \times 10^{-6} T^2 + 92.975 T^{-1} + 2.497 \times 10^{-3} T \end{aligned} \\ 553-1033 \text{ K: } \begin{aligned} \Delta H_r^\circ &= 48.055 - 1.490 \times 10^{-3} T - 0.845 \times 10^{-6} T^2 + 33.950 T^{-1} \\ \Delta G_r^\circ &= 48.055 + 1.490 \times 10^{-3} T \ln T + 0.845 \times 10^{-6} T^2 + 16.975 T^{-1} - 30.282 \times 10^{-3} T \end{aligned} \\ 1033-1097 \text{ K: } \begin{aligned} \Delta H_r^\circ &= 49.410 - 3.902 \times 10^{-3} T - 0.151 \times 10^{-6} T^2 + 11.250 T^{-1} \\ \Delta G_r^\circ &= 49.410 + 3.902 \times 10^{-3} T \ln T + 0.151 \times 10^{-6} T^2 + 5.625 T^{-1} - 47.606 \times 10^{-3} T \end{aligned} \\ 1097-1467 \text{ K: } \begin{aligned} \Delta H_r^\circ &= 47.740 - 4.048 \times 10^{-3} T - 0.151 \times 10^{-6} T^2 + 11.250 T^{-1} \\ \Delta G_r^\circ &= 47.740 + 4.048 \times 10^{-3} T \ln T + 0.151 \times 10^{-6} T^2 + 5.625 T^{-1} - 47.106 \times 10^{-3} T \end{aligned} \\ 1467-2000 \text{ K: } \begin{aligned} \Delta H_r^\circ &= 11.339 - 0.230 \times 10^{-3} T - 0.151 \times 10^{-6} T^2 + 11.250 T^{-1} \\ \Delta G_r^\circ &= 11.339 + 0.230 \times 10^{-3} T \ln T + 0.151 \times 10^{-6} T^2 + 5.625 T^{-1} + 5.545 \times 10^{-3} T \end{aligned} \end{aligned}$$

Source: Data from Mills (80) who estimated all except enthalpy of formation at 298 K.

ZnS(cubic)
Zinc Sulfide, Sphalerite
[Formation: $\text{Zn(c,l)} + \text{S(c,l)} = \text{ZnS(c)}]$

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_f°	ΔG_f°	
298.15	10.936	14.019	14.019	0	-48.790	-47.719	34.979
300	10.952	14.087	14.020	.020	-48.791	-47.712	34.758
368.3	11.381	16.386	14.252	.786	-48.829	-47.463	28.164
368.3	11.381	16.386	14.252	.786	-48.925	-47.463	28.164
388.36	11.507	16.993	14.378	1.016	-48.939	-47.382	26.664
388.36	11.507	16.993	14.378	1.016	-49.352	-47.382	26.664
400	11.580	17.334	14.459	1.150	-49.379	-47.323	25.856
432.02	11.695	18.230	14.706	1.523	-49.472	-47.155	23.855
500	11.940	19.959	15.303	2.328	-49.778	-46.764	20.440
600	12.195	22.160	16.268	3.535	-50.094	-46.130	16.803
692.73	12.385	23.926	17.177	4.675	-50.342	-45.501	14.355
692.73	12.385	23.926	17.177	4.675	-52.092	-45.501	14.355
700	12.400	24.055	17.248	4.765	-52.114	-45.431	14.184
717.824	12.432	24.367	17.421	4.986	-52.163	-45.260	13.780

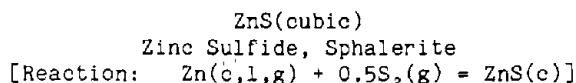
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 692.73 K, melting point of Zn; $\Delta H^\circ = 1.750$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-1300 K: $C_p^\circ = 11.700 + 1.298 \times 10^{-3}T - 1.023 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 11.700 \times 10^{-3}T + 0.649 \times 10^{-6}T^2 + 1.023 \times 10^{-2}T^3 - 3.889$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -48.271 - 1.573 \times 10^{-3}T + 0.974 \times 10^{-6}T^2 - 40.700T^{-1}$
 $\Delta G_f^\circ = -48.271 + 1.573 \times 10^{-3}T \ln T - 0.974 \times 10^{-6}T^2 - 20.350T^{-1} - 6.591 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -49.386 + 0.690 \times 10^{-3}T - 0.772 \times 10^{-6}T^2 + 114.900T^{-1}$
 $\Delta G_f^\circ = -49.386 - 0.690 \times 10^{-3}T \ln T + 0.772 \times 10^{-6}T^2 + 57.450T^{-1} + 8.591 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -65.545 + 45.430 \times 10^{-3}T - 44.054 \times 10^{-6}T^2 + 2017.100T^{-1}$
 $\Delta G_f^\circ = -65.545 - 45.430 \times 10^{-3}T \ln T + 44.054 \times 10^{-6}T^2 + 1008.550T^{-1} + 293.820 \times 10^{-3}T$
 432.02-692.73 K: $\Delta H_f^\circ = -75.023 + 41.524 \times 10^{-3}T - 24.242 \times 10^{-6}T^2 + 5243.600T^{-1}$
 $\Delta G_f^\circ = -75.023 - 41.524 \times 10^{-3}T \ln T + 24.242 \times 10^{-6}T^2 + 2621.800T^{-1} + 291.972 \times 10^{-3}T$
 692.73-717.824 K: $\Delta H_f^\circ = -75.760 + 39.123 \times 10^{-3}T - 22.850 \times 10^{-6}T^2 + 5231.000T^{-1}$
 $\Delta G_f^\circ = -75.760 - 39.123 \times 10^{-3}T \ln T + 22.850 \times 10^{-6}T^2 + 2615.500T^{-1} + 278.309 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	$H^\circ - H_{298}^\circ$	ΔH_r°	ΔG_r°	
298.15	10.936	14.019	14.019	0	-64.145	-57.233	41.952
300	10.952	14.087	14.020	.020	-64.143	-57.189	41.662
400	11.580	17.334	14.459	1.150	-64.030	-54.889	29.989
500	11.940	19.959	15.303	2.328	-63.906	-52.617	22.998
600	12.195	22.160	16.268	3.535	-63.789	-50.371	18.347
692.73	12.385	23.926	17.177	4.675	-63.693	-48.306	15.240
692.73	12.385	23.926	17.177	4.675	-65.443	-48.306	15.240
700	12.400	24.055	17.248	4.765	-65.439	-48.126	15.026
800	12.579	25.723	18.205	6.014	-65.376	-45.657	12.473
900	12.742	27.214	19.125	7.280	-65.299	-43.197	10.490
1000	12.896	28.565	20.003	8.562	-65.211	-40.747	8.905
1100	13.044	29.801	20.838	9.859	-65.112	-38.305	7.610
1180	13.158	30.721	21.477	10.908	-65.023	-36.354	6.733
1180	13.158	30.721	21.477	10.908	-92.588	-36.354	6.733
1200	13.187	30.942	21.633	11.171	-92.516	-35.403	6.448
1300	13.327	32.003	22.390	12.497	-92.141	-30.660	5.154

Phase changes: 692.73 K, melting point of Zn; $\Delta H^\circ = 1.750$ kcal/mol.
1180 K, boiling point of Zn; $\Delta H^\circ = 27.565$ kcal/mol.

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

298.15-1300 K: $C_p^\circ = 11.700 + 1.298 \times 10^{-3}T - 1.023 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 11.700 \times 10^{-3}T + 0.649 \times 10^{-6}T^2 + 1.023 \times 10^{-2}T^{-1} - 3.889$

Reaction equations (kcal/mol):

298.15-692.73 K: $\Delta H_r^\circ = -65.060 + 2.429 \times 10^{-3}T - 0.903 \times 10^{-6}T^2 + 80.750T^{-1}$
 $\Delta G_r^\circ = -65.060 - 2.429 \times 10^{-3}T \ln T + 0.903 \times 10^{-6}T^2 + 40.375T^{-1} + 39.372 \times 10^{-3}T$
692.73-1180 K: $\Delta H_r^\circ = -65.796 + 0.028 \times 10^{-3}T + 0.489 \times 10^{-6}T^2 + 68.150T^{-1}$
 $\Delta G_r^\circ = -65.796 - 0.028 \times 10^{-3}T \ln T - 0.489 \times 10^{-6}T^2 + 34.075T^{-1} + 25.708 \times 10^{-3}T$
1180-1300 K: $\Delta H_r^\circ = -96.349 + 2.560 \times 10^{-3}T + 0.489 \times 10^{-6}T^2 + 68.150T^{-1}$
 $\Delta G_r^\circ = -96.349 - 2.560 \times 10^{-3}T \ln T - 0.489 \times 10^{-6}T^2 + 34.075T^{-1} + 69.510 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Schaefer (103). Low-temperature heat capacities and entropy at 298 K from Stuve (111). High-temperature data based on Pankratz (93).

ZnS(hexagonal)
Zinc Sulfide, Wurtzite
[Formation: $\text{Zn(c,l)} + \text{S(c,l)} = \text{ZnS(c)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H _{2,98} °)/T	H°- H _{2,98} °	ΔHf°	ΔGf°	
298.15	10.965	14.064	14.064	0	-46.570	-45.512	33.361
300	10.983	14.132	14.065	.020	-46.571	-45.506	33.150
368.3	11.417	16.438	14.296	.789	-46.606	-45.259	26.857
368.3	11.417	16.438	14.296	.789	-46.702	-45.259	26.857
388.36	11.545	17.047	14.423	1.019	-46.716	-45.180	25.425
388.36	11.545	17.047	14.423	1.019	-47.129	-45.180	25.425
400	11.619	17.389	14.504	1.154	-47.155	-45.121	24.653
432.02	11.733	18.288	14.752	1.528	-47.247	-44.955	22.742
500	11.975	20.023	15.353	2.335	-47.551	-44.569	19.481
600	12.222	22.230	16.320	3.546	-47.863	-43.941	16.005
692.73	12.404	23.999	17.232	4.688	-48.109	-43.319	13.667
692.73	12.404	23.999	17.232	4.688	-49.859	-43.319	13.667
700	12.418	24.129	17.303	4.778	-49.881	-43.250	13.503
717.824	12.448	24.442	17.477	5.000	-49.930	-43.080	13.116

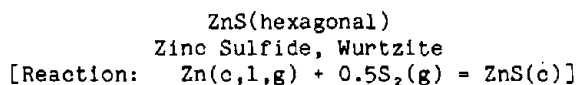
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 692.73 K, melting point of Zn; $\Delta H^\circ = 1.750$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n (n = 1 to 8).

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

298.15-1300 K: $C_p^\circ = 11.819 + 1.166 \times 10^{-3}T - 1.067 \times 10^{-5}T^2$
 $H^\circ - H_{2,98}^\circ = 11.819 \times 10^{-3}T + 0.583 \times 10^{-6}T^2 + 1.067 \times 10^{-2}T^{-1} - 3.934$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = -46.095 - 1.454 \times 10^{-3}T + 0.908 \times 10^{-6}T^2 - 36.300T^{-1}$
 $\Delta G_f^\circ = -46.095 + 1.454 \times 10^{-3}T \ln T - 0.908 \times 10^{-6}T^2 - 18.150T^{-1} - 5.854 \times 10^{-3}T$
 368.3-388.36 K: $\Delta H_f^\circ = -47.211 + 0.809 \times 10^{-3}T - 0.838 \times 10^{-6}T^2 + 119.300T^{-1}$
 $\Delta G_f^\circ = -47.211 - 0.809 \times 10^{-3}T \ln T + 0.838 \times 10^{-6}T^2 + 59.650T^{-1} + 9.329 \times 10^{-3}T$
 388.36-432.02 K: $\Delta H_f^\circ = -63.369 + 45.549 \times 10^{-3}T - 44.120 \times 10^{-6}T^2 + 2021.500T^{-1}$
 $\Delta G_f^\circ = -63.369 - 45.549 \times 10^{-3}T \ln T + 44.120 \times 10^{-6}T^2 + 1010.750T^{-1} + 294.557 \times 10^{-3}T$
 432.02-692.73 K: $\Delta H_f^\circ = -72.848 + 41.643 \times 10^{-3}T - 24.308 \times 10^{-6}T^2 + 5248.000T^{-1}$
 $\Delta G_f^\circ = -72.848 - 41.643 \times 10^{-3}T \ln T + 24.308 \times 10^{-6}T^2 + 2624.000T^{-1} + 292.710 \times 10^{-3}T$
 692.73-717.824 K: $\Delta H_f^\circ = -73.584 + 39.242 \times 10^{-3}T - 22.916 \times 10^{-6}T^2 + 5235.400T^{-1}$
 $\Delta G_f^\circ = -73.584 - 39.242 \times 10^{-3}T \ln T + 22.916 \times 10^{-6}T^2 + 2617.700T^{-1} + 279.046 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHr°	ΔGr°	
298.15	10.965	14.064	14.064	0	-61.925	-55.026	40.335
300	10.983	14.132	14.065	.020	-61.923	-54.983	40.055
400	11.619	17.389	14.504	1.154	-61.806	-52.687	28.786
500	11.975	20.023	15.353	2.335	-61.679	-50.422	22.039
600	12.222	22.230	16.320	3.546	-61.557	-48.182	17.550
692.73	12.404	23.999	17.232	4.688	-61.460	-46.124	14.552
692.73	12.404	23.999	17.232	4.688	-63.210	-46.124	14.552
700	12.418	24.129	17.303	4.778	-63.206	-45.945	14.345
800	12.585	25.798	18.263	6.028	-63.142	-43.483	11.879
900	12.737	27.289	19.185	7.294	-63.066	-41.031	9.964
1000	12.878	28.639	20.064	8.575	-62.978	-38.588	8.433
1100	13.013	29.872	20.899	9.870	-62.881	-36.152	7.183
1180	13.118	30.789	21.539	10.915	-62.796	-34.208	6.336
1180	13.118	30.789	21.539	10.915	-90.361	-34.208	6.336
1200	13.144	31.010	21.695	11.178	-90.289	-33.258	6.057
1300	13.272	32.067	22.452	12.499	-89.919	-28.521	4.795

Phase changes: 692.73 K, melting point of Zn; ΔH° = 1.750 kcal/mol.
1180 K, boiling point of Zn; ΔH° = 27.565 kcal/mol.

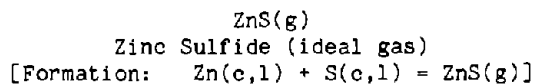
Heat capacity (cal/mol·K) and enthalpy (kcal/mol) equations:

298.15-1300 K: $\text{Cp}^\circ = 11.819 + 1.166 \times 10^{-3}T - 1.067 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}_{298}^\circ = 11.819 \times 10^{-3}T + 0.583 \times 10^{-6}T^2 + 1.067 \times 10^{-2}T^{-1} - 3.934$

Reaction equations (kcal/mol):

298.15-692.73 K: $\Delta \text{Hr}^\circ = -62.884 + 2.549 \times 10^{-3}T - 0.969 \times 10^{-6}T^2 + 85.150T^{-1}$
 $\Delta \text{Gr}^\circ = -62.884 - 2.549 \times 10^{-3}T \ln T + 0.969 \times 10^{-6}T^2 + 42.575T^{-1} + 40.109 \times 10^{-3}T$
692.73-1180 K: $\Delta \text{Hr}^\circ = -63.621 + 0.148 \times 10^{-3}T + 0.423 \times 10^{-6}T^2 + 72.550T^{-1}$
 $\Delta \text{Gr}^\circ = -63.621 - 0.148 \times 10^{-3}T \ln T - 0.423 \times 10^{-6}T^2 + 36.275T^{-1} + 26.446 \times 10^{-3}T$
1180-1300 K: $\Delta \text{Hr}^\circ = -94.174 + 2.679 \times 10^{-3}T + 0.423 \times 10^{-6}T^2 + 72.550T^{-1}$
 $\Delta \text{Gr}^\circ = -94.174 - 2.679 \times 10^{-3}T \ln T - 0.423 \times 10^{-6}T^2 + 36.275T^{-1} + 70.247 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K from Adami (1). Low-temperature heat capacities and entropy at 298 K from Stuve (111). High-temperature data based on Pankratz (93).



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15	8.456	56.835	56.835	0	48.600	36.905	-27.052
300	8.461	56.887	56.835	.016	48.595	36.834	-26.833
368.3	8.606	58.641	57.011	.600	48.375	34.179	-20.282
368.3	8.606	58.641	57.011	.600	48.279	34.179	-20.282
388.36	8.649	59.098	57.107	.773	48.208	33.413	-18.803
388.36	8.649	59.098	57.107	.773	47.795	33.413	-18.803
400	8.674	59.354	57.169	.874	47.735	32.983	-18.021
432.02	8.711	60.023	57.356	1.152	47.548	31.809	-16.091
500	8.789	61.303	57.809	1.747	47.031	29.374	-12.839
600	8.859	62.912	58.529	2.630	46.391	25.904	-9.435
692.73	8.904	64.188	59.203	3.453	45.826	22.777	-7.186
692.73	8.904	64.188	59.203	3.453	44.076	22.777	-7.186
700	8.907	64.281	59.255	3.518	44.029	22.554	-7.041
717.824	8.913	64.505	59.383	3.677	43.917	22.009	-6.701

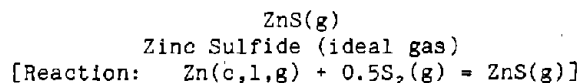
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
 388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
 432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
 692.73 K, melting point of Zn; $\Delta H^\circ = 1.750$ kcal/mol.
 717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-3000 K: $\text{Cp}^\circ = 8.909 + 0.120 \times 10^{-3}T - 0.434 \times 10^{-5}T^2$
 $\text{H}^\circ - \text{H}^\circ_{298} = 8.909 \times 10^{-3}T + 0.060 \times 10^{-6}T^2 + 0.434 \times 10^{-2}T^{-1} - 2.807$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta \text{Hf}^\circ = 50.201 - 4.364 \times 10^{-3}T + 0.385 \times 10^{-6}T^2 - 99.600T^{-1}$
 $\Delta \text{Gf}^\circ = 50.201 + 4.364 \times 10^{-3}T \ln T - 0.385 \times 10^{-6}T^2 - 49.800T^{-1} - 68.783 \times 10^{-3}T$
 368.3-388.36 K: $\Delta \text{Hf}^\circ = 49.086 - 2.101 \times 10^{-3}T - 1.361 \times 10^{-6}T^2 + 56.000T^{-1}$
 $\Delta \text{Gf}^\circ = 49.086 + 2.101 \times 10^{-3}T \ln T + 1.361 \times 10^{-6}T^2 + 28.000T^{-1} - 53.600 \times 10^{-3}T$
 388.36-432.02 K: $\Delta \text{Hf}^\circ = 32.928 + 42.639 \times 10^{-3}T - 44.643 \times 10^{-6}T^2 + 1958.200T^{-1}$
 $\Delta \text{Gf}^\circ = 32.928 - 42.639 \times 10^{-3}T \ln T + 44.643 \times 10^{-6}T^2 + 979.100T^{-1} + 231.628 \times 10^{-3}T$
 432.02-692.73 K: $\Delta \text{Hf}^\circ = 23.449 + 38.733 \times 10^{-3}T - 24.831 \times 10^{-6}T^2 + 5184.700T^{-1}$
 $\Delta \text{Gf}^\circ = 23.449 - 38.733 \times 10^{-3}T \ln T + 24.831 \times 10^{-6}T^2 + 2592.350T^{-1} + 229.781 \times 10^{-3}T$
 692.73-717.824 K: $\Delta \text{Hf}^\circ = 22.712 + 36.332 \times 10^{-3}T - 23.439 \times 10^{-6}T^2 + 5172.100T^{-1}$
 $\Delta \text{Gf}^\circ = 22.712 - 36.332 \times 10^{-3}T \ln T + 23.439 \times 10^{-6}T^2 + 2586.050T^{-1} + 216.117 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15	8.456	56.835	56.835	0	33.245	27.392	-20.078
300	8.461	56.887	56.835	.016	33.243	27.357	-19.929
400	8.674	59.354	57.169	.874	33.084	25.417	-13.887
500	8.789	61.303	57.809	1.747	32.903	23.520	-10.281
600	8.859	62.912	58.529	2.630	32.697	21.663	-7.891
692.73	8.904	64.188	59.203	3.453	32.476	19.971	-6.301
692.73	8.904	64.188	59.203	3.453	30.726	19.971	-6.301
700	8.907	64.281	59.255	3.518	30.704	19.859	-6.200
800	8.942	65.473	59.959	4.411	30.411	18.330	-5.008
900	8.970	66.528	60.631	5.307	30.117	16.837	-4.089
1000	8.993	67.474	61.269	6.205	29.822	15.378	-3.361
1100	9.013	68.332	61.873	7.105	29.524	13.947	-2.771
1180	9.027	68.965	62.333	7.826	29.285	12.826	-2.375
1180	9.027	68.965	62.333	7.826	1.720	12.826	-2.375
1200	9.030	69.117	62.444	8.007	1.710	13.013	-2.370
1300	9.046	69.841	62.986	8.911	1.663	13.954	-2.346
1400	9.061	70.512	63.501	9.816	1.612	14.903	-2.326
1500	9.075	71.137	63.988	10.723	1.560	15.853	-2.310
1600	9.089	71.723	64.454	11.631	1.506	16.808	-2.296
1700	9.102	72.275	64.898	12.541	1.450	17.765	-2.284
1800	9.114	72.795	65.322	13.452	1.391	18.728	-2.274
1900	9.126	73.288	65.728	14.364	1.331	19.694	-2.265
2000	9.138	73.757	66.119	15.277	1.268	20.658	-2.257

Phase changes: 692.73 K, melting point of Zn; ΔH° = 1.750 kcal/mol.
1180 K, boiling point of Zn; ΔH° = 27.565 kcal/mol.

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

298.15-3000 K: $C_p^\circ = 8.909 + 0.120 \times 10^{-3}T - 0.434 \times 10^{-5}T^2$
 $H^\circ - H_{298}^\circ = 8.909 \times 10^{-3}T + 0.060 \times 10^{-6}T^2 + 0.434 \times 10^{-2}T^{-1} - 2.807$

Reaction equations (kcal/mol):

298.15-692.73 K: $\Delta H_r^\circ = 33.412 - 0.362 \times 10^{-3}T - 1.492 \times 10^{-6}T^2 + 21.850T^{-1}$
 $\Delta G_r^\circ = 33.412 + 0.362 \times 10^{-3}T \ln T + 1.492 \times 10^{-6}T^2 + 10.925T^{-1} - 22.820 \times 10^{-3}T$
692.73-1180 K: $\Delta H_r^\circ = 32.676 - 2.763 \times 10^{-3}T - 0.100 \times 10^{-6}T^2 + 9.250T^{-1}$
 $\Delta G_r^\circ = 32.676 + 2.763 \times 10^{-3}T \ln T + 0.100 \times 10^{-6}T^2 + 4.625T^{-1} - 36.483 \times 10^{-3}T$
1180-2000 K: $\Delta H_r^\circ = 2.123 - 0.231 \times 10^{-3}T - 0.100 \times 10^{-6}T^2 + 9.250T^{-1}$
 $\Delta G_r^\circ = 2.123 + 0.231 \times 10^{-3}T \ln T + 0.100 \times 10^{-6}T^2 + 4.625T^{-1} + 7.318 \times 10^{-3}T$

Sources: Enthalpy of formation at 298 K based on Ban (4) and Piacente (99). Other data based on Marquart (77).

ZrS(g)
Zirconium Monosulfide (ideal gas)
[Formation: $\text{Zr(c)} + \text{S(c,l)} = \text{ZrS(g)}$]

T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHf°	ΔGf°	
298.15*	8.000	59.000	59.000	0	74.000	61.472	-45.060
300	8.010	59.050	59.000	.015	73.994	61.395	-44.726
368.3	8.263	60.733	59.174	.574	73.735	58.551	-34.744
368.3	8.263	60.733	59.174	.574	73.639	58.551	-34.744
388.36	8.337	61.173	59.266	.741	73.557	57.732	-32.488
388.36	8.337	61.173	59.266	.741	73.144	57.732	-32.488
400	8.380	61.420	59.325	.838	73.077	57.271	-31.291
432.02	8.434	62.067	59.505	1.107	72.872	56.013	-28.335
500	8.550	63.310	59.940	1.685	72.320	53.405	-23.343
600	8.650	64.880	60.637	2.546	71.632	49.688	-18.098
700	8.710	66.210	61.331	3.415	70.988	46.088	-14.389
717.824	8.719	66.429	61.455	3.570	70.877	45.456	-13.840

*Data except enthalpy of formation at 298 K estimated.

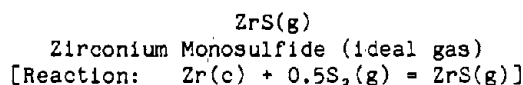
Phase changes: 368.3 K, orthorhombic - monoclinic transition point of S; $\Delta H^\circ = 0.096$ kcal/mol.
388.36 K, melting point of S; $\Delta H^\circ = 0.413$ kcal/mol.
432.02 K, second order transformation of S; $\Delta H^\circ = 0$ kcal/mol.
717.824 K, boiling point of S to equilibrium mixture of S_n ($n = 1$ to 8).

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

298.15-2000 K: $C_p^\circ = 8.828 + 0.058 \times 10^{-3}T - 0.751 \times 10^{-5}T^{-2}$
 $H^\circ - H_{298}^\circ = 8.828 \times 10^{-3}T + 0.029 \times 10^{-6}T^2 + 0.751 \times 10^{-2}T^{-1} - 2.887$

Formation equations (kcal/mol):

298.15-368.3 K: $\Delta H_f^\circ = 75.901 - 5.339 \times 10^{-3}T + 0.804 \times 10^{-6}T^2 - 113.400T^{-1}$
 $\Delta G_f^\circ = 75.901 + 5.339 \times 10^{-3}T \ln T - 0.804 \times 10^{-6}T^2 - 56.700T^{-1} - 77.936 \times 10^{-3}T$
368.3-388.36 K: $\Delta H_f^\circ = 74.786 - 3.076 \times 10^{-3}T - 0.942 \times 10^{-6}T^2 + 42.200T^{-1}$
 $\Delta G_f^\circ = 74.786 + 3.076 \times 10^{-3}T \ln T + 0.942 \times 10^{-6}T^2 + 21.100T^{-1} - 62.753 \times 10^{-3}T$
388.36-432.02 K: $\Delta H_f^\circ = 58.627 + 41.664 \times 10^{-3}T - 44.224 \times 10^{-6}T^2 + 1944.400T^{-1}$
 $\Delta G_f^\circ = 58.627 - 41.664 \times 10^{-3}T \ln T + 44.224 \times 10^{-6}T^2 + 972.200T^{-1} + 222.475 \times 10^{-3}T$
432.02-717.824 K: $\Delta H_f^\circ = 49.149 + 37.758 \times 10^{-3}T - 24.412 \times 10^{-6}T^2 + 5170.900T^{-1}$
 $\Delta G_f^\circ = 49.149 - 37.758 \times 10^{-3}T \ln T + 24.412 \times 10^{-6}T^2 + 2585.450T^{-1} + 220.628 \times 10^{-3}T$



T, K	cal/mol·K			kcal/mol			Log Kr
	Cp°	S°	-(G° - H° ₂₉₈)/T	H° - H° ₂₉₈	ΔHr°	ΔGr°	
298.15*	8.000	59.000	59.000	0	58.645	51.958	-38.086
300	8.010	59.050	59.000	.015	58.642	51.918	-37.821
400	8.380	61.420	59.325	.838	58.426	49.705	-27.157
500	8.550	63.310	59.940	1.685	58.192	47.552	-20.785
600	8.650	64.880	60.637	2.546	57.938	45.447	-16.554
700	8.710	66.210	61.331	3.415	57.663	43.393	-13.548
800	8.760	67.380	62.020	4.288	57.366	41.371	-11.302
900	8.790	68.410	62.671	5.165	57.049	39.393	-9.566
1000	8.810	69.340	63.295	6.045	56.710	37.447	-8.184
1100	8.830	70.180	63.883	6.927	56.351	35.539	-7.061
1136	8.834	70.464	64.087	7.245	56.216	34.859	-6.706
1136	8.834	70.464	64.087	7.245	55.265	34.859	-6.706
1200	8.840	70.950	64.441	7.811	55.110	33.714	-6.140
1300	8.860	71.660	64.971	8.696	54.854	31.938	-5.369
1400	8.870	72.320	65.476	9.582	54.580	30.182	-4.712
1500	8.880	72.930	65.950	10.470	54.287	28.453	-4.146
1600	8.890	73.500	66.401	11.358	53.974	26.745	-3.653
1700	8.900	74.040	66.835	12.248	53.644	25.052	-3.221
1800	8.910	74.550	67.251	13.138	53.295	23.378	-2.838
1900	8.920	75.030	67.646	14.030	52.928	21.729	-2.499
2000	8.930	75.490	68.029	14.922	52.542	20.093	-2.196

*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: $\text{Cp}^\circ = 8.828 + 0.058 \times 10^{-3}T - 0.751 \times 10^{-5}T^{-2}$
 $\text{H}^\circ - \text{H}^\circ_{298} = 8.828 \times 10^{-3}T + 0.029 \times 10^{-6}T^2 + 0.751 \times 10^{-2}T^{-1} - 2.887$

Reaction equations (kcal/mol):

298.15-1136 K: $\Delta\text{Hr}^\circ = 59.112 - 1.337 \times 10^{-3}T - 1.073 \times 10^{-6}T^2 + 8.050T^{-1}$
 $\Delta\text{Gr}^\circ = 59.112 + 1.337 \times 10^{-3}T \ln T + 1.073 \times 10^{-6}T^2 + 4.025T^{-1} - 31.973 \times 10^{-3}T$
 1136-2000 K: $\Delta\text{Hr}^\circ = 56.616 - 0.168 \times 10^{-3}T - 0.942 \times 10^{-6}T^2 + 62.550T^{-1}$
 $\Delta\text{Gr}^\circ = 56.616 + 0.168 \times 10^{-3}T \ln T + 0.942 \times 10^{-6}T^2 + 31.275T^{-1} - 21.424 \times 10^{-3}T$

Source: Data from Mills (80) who estimated all except enthalpy of formation at 298 K.

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