

$H_2(g)$
Hydrogen

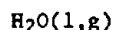
T, K	cal/mol·K			$H^\circ - H_{298}^\circ$, kcal/mol
	C_p°	S°	$-(G^\circ - H_{298}^\circ)/T$	
298.15	6.892	31.207	31.207	0
300	6.895	31.250	31.207	.013
400	6.974	33.247	31.480	.707
500	6.993	34.806	31.994	1.406
600	7.009	36.082	32.572	2.106
700	7.036	37.164	33.153	2.808
800	7.080	38.107	33.715	3.514
900	7.142	38.944	34.250	4.225
1000	7.219	39.700	34.757	4.943
1100	7.309	40.392	35.238	5.669
1200	7.407	41.033	35.695	6.405
1300	7.510	41.630	36.129	7.151
1400	7.615	42.190	36.542	7.907
1500	7.719	42.719	36.936	8.674
1600	7.821	43.220	37.313	9.451
1700	7.920	43.698	37.676	10.238
1800	8.016	44.153	38.022	11.035
1900	8.106	44.589	38.357	11.841
2000	8.193	45.007	38.679	12.656
2100	8.275	45.409	38.990	13.479
2200	8.354	45.795	39.290	14.311
2300	8.428	46.168	39.581	15.150
2400	8.499	46.529	39.864	15.996
2500	8.566	46.877	40.137	16.849
2600	8.631	47.214	40.403	17.709
2700	8.692	47.541	40.661	18.575
2800	8.752	47.858	40.912	19.448
2900	8.809	48.166	41.157	20.326
3000	8.864	48.466	41.396	21.209

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

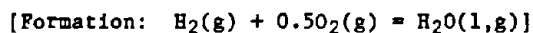
$$298.15\text{--}3000\text{ K: } C_p^\circ = 6.456 + 0.838 \times 10^{-3}T + 0.165 \times 10^{-5}T^2$$

$$H^\circ - H_{298}^\circ = 6.456 \times 10^{-3}T + 0.419 \times 10^{-6}T^2 - 0.165 \times 10^{-2}T^{-1} - 1.907$$

Source: Data from JANAF (52).



Water



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G°- H ₂₉₈ °)/T	H°- H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	17.997	16.718	16.718	0	-68.315	-56.690	41.554
300	17.995	16.829	16.719	.033	-68.302	-56.618	41.246
373.15	18.153	20.765	17.139	1.353	-67.747	-53.831	31.528
373.15	8.134	46.921	17.139	11.113	-57.987	-53.831	31.528
400	8.186	47.484	19.124	11.344	-58.040	-53.516	29.240
500	8.415	49.334	24.988	12.173	-58.275	-52.359	22.886
600	8.676	50.891	29.178	13.028	-58.498	-51.154	18.633
700	8.954	52.249	32.379	13.909	-58.708	-49.913	15.583
800	9.246	53.464	34.940	14.819	-58.903	-48.644	13.289
900	9.547	54.570	37.060	15.759	-59.081	-47.350	11.498
1000	9.851	55.592	38.864	16.728	-59.243	-46.040	10.062
1100	10.152	56.545	40.428	17.729	-59.388	-44.711	8.883
1200	10.444	57.441	41.809	18.759	-59.518	-43.370	7.899
1300	10.723	58.288	43.044	19.817	-59.634	-42.020	7.064
1400	10.987	59.092	44.161	20.903	-59.736	-40.661	6.347
1500	11.233	59.859	45.183	22.014	-59.827	-39.297	5.725
1600	11.462	60.591	46.123	23.149	-59.907	-37.925	5.180
1700	11.674	61.293	46.995	24.306	-59.978	-36.549	4.699
1800	11.869	61.965	47.808	25.483	-60.042	-35.168	4.270
1900	12.048	62.612	48.570	26.679	-60.099	-33.785	3.886
2000	12.214	63.234	49.288	27.892	-60.151	-32.399	3.540
2100	12.366	63.834	49.967	29.121	-60.197	-31.009	3.227
2200	12.505	64.412	50.610	30.365	-60.240	-29.619	2.942
2300	12.634	64.971	51.222	31.622	-60.280	-28.227	2.682
2400	12.753	65.511	51.806	32.891	-60.318	-26.830	2.443
2500	12.863	66.034	52.365	34.172	-60.353	-25.435	2.223
2600	12.965	66.541	52.901	35.464	-60.386	-24.039	2.021
2700	13.059	67.032	53.415	36.765	-60.419	-22.641	1.833
2800	13.146	67.508	53.910	38.075	-60.453	-21.240	1.658
2900	13.228	67.971	54.387	39.394	-60.485	-19.840	1.495
3000	13.304	68.421	54.848	40.720	-60.517	-18.437	1.343

Phase changes: 273.15 K, melting point of H₂O; ΔH° = 1.436 kcal/mol.

373.15 K, boiling point of H₂O; ΔH° = 9.760 kcal/mol.

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

298.15-373.15 K: Cp° = 18.041

$$\text{H}^\circ - \text{H}_{298}^\circ = 18.041 \times 10^{-3} T - 5.379$$

373.15-3000 K: Cp° = 7.272 + 2.492 × 10⁻³ T - 0.094 × 10⁻⁵ T²

$$\text{H}^\circ - \text{H}_{298}^\circ = 7.272 \times 10^{-3} T + 1.246 \times 10^{-6} T^2 + 0.094 \times 10^{-2} T^{-1} + 8.201$$

H₂O(l,g) - ContinuedFormation equations (kcal/mol):

$$298.15-373.15 \text{ K: } \Delta H_f^\circ = -70.611 + 7.970 \times 10^{-3} T - 0.671 \times 10^{-6} T^2 - 6.100 T^{-1}$$

$$\Delta G_f^\circ = -70.611 - 7.970 \times 10^{-3} T \ln T + 0.671 \times 10^{-6} T^2 - 3.050 T^{-1} + 91.937 \times 10^{-3} T$$

$$373.15-2000 \text{ K: } \Delta H_f^\circ = -57.031 - 2.799 \times 10^{-3} T + 0.576 \times 10^{-6} T^2 + 3.300 T^{-1}$$

$$\Delta G_f^\circ = -57.031 + 2.799 \times 10^{-3} T \ln T - 0.576 \times 10^{-6} T^2 + 1.650 T^{-1} - 7.798 \times 10^{-3} T$$

$$2000-3000 \text{ K: } \Delta H_f^\circ = -56.363 - 3.354 \times 10^{-3} T + 0.722 \times 10^{-6} T^2 - 289.100 T^{-1}$$

$$\Delta G_f^\circ = -56.363 + 3.354 \times 10^{-3} T \ln T - 0.722 \times 10^{-6} T^2 - 144.550 T^{-1} - 12.020 \times 10^{-3} T$$

Sources: Enthalpy of formation at 298 K for liquid and gas from CODATA (36). Entropy at 298 K for liquid also from CODATA (36). Data for liquid from Ginnings (77). Data for gas from JANAF (51).



Water (ideal gas)



T, K	cal/mol·K			kcal/mol			Log Kf
	Cp°	S°	-(G° - H ₂₉₈ °)/T	H° - H ₂₉₈ °	ΔHf°	ΔGf°	
298.15	8.025	45.106	45.106	0	-57.795	-54.634	40.047
300	8.027	45.155	45.106	.015	-57.799	-54.614	39.786
400	8.186	47.484	45.422	.825	-58.038	-53.515	29.239
500	8.415	49.334	46.026	1.654	-58.274	-52.358	22.885
600	8.676	50.891	46.709	2.509	-58.496	-51.153	18.632
700	8.954	52.249	47.406	3.390	-58.707	-49.912	15.583
800	9.246	53.464	48.089	4.300	-58.902	-48.643	13.289
900	9.547	54.570	48.748	5.240	-59.080	-47.349	11.498
1000	9.851	55.592	49.383	6.209	-59.242	-46.039	10.062
1100	10.152	56.545	49.990	7.210	-59.387	-44.710	8.883
1200	10.444	57.441	50.574	8.240	-59.517	-43.369	7.899
1300	10.723	58.288	51.136	9.298	-59.632	-42.019	7.064
1400	10.987	59.092	51.675	10.384	-59.735	-40.660	6.347
1500	11.233	59.859	52.196	11.495	-59.826	-39.296	5.725
1600	11.462	60.591	52.697	12.630	-59.906	-37.924	5.180
1700	11.674	61.293	53.183	13.787	-59.977	-36.548	4.698
1800	11.869	61.965	53.652	14.964	-60.041	-35.167	4.270
1900	12.048	62.612	54.107	16.160	-60.098	-33.784	3.886
2000	12.214	63.234	54.548	17.373	-60.150	-32.398	3.540

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

298.15-2000 K: $C_p^\circ = 6.895 + 2.882 \times 10^{-3}T + 0.240 \times 10^{-5}T^{-2}$

$H^\circ - H_{298}^\circ = 6.895 \times 10^{-3}T + 1.441 \times 10^{-6}T^2 - 0.240 \times 10^{-2}T^{-1} - 2.103$

Formation equations (kcal/mol):

298.15-2000 K: $\Delta H_f^\circ = -56.816 - 3.176 \times 10^{-3}T + 0.771 \times 10^{-6}T^2 - 30.100T^{-1}$

$\Delta G_f^\circ = -56.816 + 3.176 \times 10^{-3}T \ln T - 0.771 \times 10^{-6}T^2 - 15.050T^{-1} - 10.378 \times 10^{-3}T$

Sources: Enthalpy of formation and entropy at 298 K from CODATA (36). All other data from JANAF (51).

O₂(g)

Oxygen

T, K	cal/mol·K			H° - H° ₂₉₈ ,
	Cp°	S°	-(G° - H° ₂₉₈)/T	kcal/mol
298.15	7.021	49.005	49.005	0
300	7.023	49.049	49.006	.013
400	7.196	51.090	49.283	.723
500	7.431	52.721	49.813	1.454
600	7.670	54.097	50.415	2.209
700	7.883	55.296	51.029	2.987
800	8.062	56.360	51.629	3.785
900	8.211	57.319	52.209	4.599
1000	8.334	58.190	52.764	5.426
1100	8.437	58.990	53.295	6.265
1200	8.525	59.728	53.801	7.113
1300	8.601	60.413	54.283	7.969
1400	8.670	61.053	54.744	8.833
1500	8.734	61.653	55.184	9.703
1600	8.795	62.219	55.607	10.580
1700	8.853	62.754	56.012	11.462
1800	8.909	63.262	56.401	12.350
1900	8.965	63.745	56.774	13.244
2000	9.020	64.206	57.135	14.143
2100	9.075	64.648	57.482	15.048
2200	9.129	65.071	57.817	15.958
2300	9.182	65.478	58.141	16.874
2400	9.235	65.870	58.455	17.795
2500	9.287	66.248	58.760	18.721
2600	9.337	66.613	59.055	19.652
2700	9.387	66.966	59.341	20.588
2800	9.435	67.309	59.620	21.529
2900	9.482	67.641	59.891	22.475
3000	9.528	67.963	60.154	23.426

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

$$298.15\text{--}2000\text{ K: } Cp^\circ = 7.230 + 1.006 \times 10^{-3}T - 0.452 \times 10^{-5}T^{-2}$$

$$H^\circ - H^\circ_{298} = 7.230 \times 10^{-3}T + 0.503 \times 10^{-6}T^2 + 0.452 \times 10^2 T^{-1} - 2.352$$

$$2000\text{--}3000\text{ K: } Cp^\circ = 8.340 + 0.418 \times 10^{-3}T - 6.300 \times 10^{-5}T^{-2}$$

$$H^\circ - H^\circ_{298} = 8.340 \times 10^{-3}T + 0.209 \times 10^{-6}T^2 + 6.300 \times 10^2 T^{-1} - 3.688$$

Source: Data from JANAF (52).