Water (H₂O) LIQUID, p = 1 BAR M_r = 18.01528 Water (H₂O) H_2O_1(l)

$S°$(298.15 K) = 69.950 ± 0.079 $J \cdot K^{-1} \cdot mol^{-1}$ $\Delta_f H°$(298.15 K) = −285.830 ± 0.042 $kJ \cdot mol^{-1}$

| | | Enthalpy Reference Temperature = T_r = 298.15 K | | | | Standard State Pressure = $p°$ = 0.1 MPa | |
| | $J \cdot K^{-1} \cdot mol^{-1}$ | | | $kJ \cdot mol^{-1}$ | | | |
T/K	$C_p°$	$S°$	$-(G°-H°(T_r))/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
280	75.563	65.215	70.102	−1.368	−286.410	−240.123	44.796
298.15	75.351	69.950	69.950	0.	−285.830	−237.141	41.546
300	75.349	70.416	69.952	0.139	−285.771	−236.839	41.237
320	75.344	75.279	70.134	1.646	−285.137	−233.598	38.131
340	75.388	79.847	70.573	3.153	−284.506	−230.396	35.396
360	75.679	84.164	71.209	4.664	−283.874	−227.231	32.970
372.780	75.962	86.808	71.699	5.633	— LIQUID <---> REAL GAS —		—
380	76.154	88.267	72.000	6.182	−283.237	−224.102	30.805
400	76.770	92.189	72.912	7.711	−282.591	−221.006	28.860
420	77.547	95.952	73.920	9.254	−281.934	−217.943	27.105
440	78.543	99.582	75.004	10.814	−281.262	−214.912	25.513
460	79.793	103.100	76.150	12.397	−280.569	−211.911	24.063
480	81.463	106.530	77.344	14.009	−279.850	−208.941	22.737
500	83.694	109.898	78.579	15.659	−279.095	−206.002	21.521

Enthalpy of Formation

The adopted enthalpy of formation and uncertainty are taken from the CODATA recommended values[1] which are, in turn, based on calorimetric measurements by Rossini[2] and King and Armstrong.[3]

Heat Capacity and Entropy

The adopted $C_p°$ data from 273.15 to 373.15 K are taken from the very accurate calorimetric measurements of Osborne et al.[4] Heat capacity data taken from the recent equation of state formulation of Haar et al.[5] agree with the adopted data to within 0.06% above 320 K with deviations up to 0.12% being noted near 305 K. In the latter region the experimental $C_p°$ data go through a single smooth minimum while data derived from the equation of state exhibit an incipient double minimum behavior. These deviations are very small and would lead to nearly negligible differences in the thermochemical functions.

We have made an approximate extrapolation of $C_p°$(l, p=1 bar) to temperatures where water is unstable with respect to vaporization by using data derived from Haar's equation of state formulation.[5] From 373.15 to 390 K the adopted $C_p°$(1 bar) data were taken directly from Haar et al.[5] while from 400 to 450 K the adopted $C_p°$ data were derived by taking advantage of the constant difference of 0.0090 $cal \cdot K^{-1} \cdot mol^{-1}$ between C_p(10 bar) and $C_p°$(1 bar) observed between 320 to 390 K using the data of Haar et al.[5] Above 450 K the C_p(100 bar) data[5] were adjusted by a similar procedure although the difference is no longer constant. The C_p adjustment from 10 bar to 1 bar is less than 0.05% while that from 100 bar to 1 bar ranges from 0.9 to 1.2%.

The adopted value of $S°$(298.15 K) = 16.718 ± 0.019 $cal \cdot K^{-1} \cdot mol^{-1}$ is taken from the CODATA recommended value.[1] This was calculated by CODATA from the entropy of the ideal gas with appropriate corrections for real gas behavior and vaporization.

Vaporization Data

The boiling point and enthalpy of vaporization to the real gas at p=1 bar are taken from the work of Haar et al.[5] see the H₂O (liquid–real gas at p=1 bar) JANAF Table[6] for further details. The enthalpy of vaporization, $\Delta_{vap}H°$, to the ideal gas is calculated as $\Delta_{vap}H° = \Delta_f H°$(g) $= \Delta_f H°$(l, p=1 bar) using JANAF data.[6] The temperature and enthalpy of vaporization at f=1 bar represent the calculated values at the point where $\Delta_f G°$ = 0 for the process H₂O(l) → H₂O(ideal gas). Thus, these values represent boiling to the (hypothetical) ideal vapor at a fugacity of 1 bar.

References

[1]ICSU CODATA Task Group, J. Chem. Thermodyn. 4, 331 (1972); see also, CODATA Bulletin #17, "CODATA Recommended Key Values for Thermodynamics 1975." (1976).

[2]F. D. Rossini, J. Res. Nat. Bur. Stand. 6, 1 (1931); ibid 6, 36 (1931); ibid 22, 407 (1939).

[3]R. King and G. T. Armstrong, J. Res. Nat. Bur. Stand. 72A, 113 (1968).

[4]N. S. Osborne, H. F. Stimson and D. C. Ginnings, J. Res. Nat. Bur. Stand. 23, 197 (1939).

[5]L. Haar, J. Gallagher and G. S. Kell, Ninth International Conference on Properties of Steam, Sept. 1979, Munich; and personal communication from L. Haar and J. Gallagher, U. S. Nat. Bur. Stand., (May 1980).

[6]JANAF Thermochemical Tables: H₂O(liquid real gas at p=1 bar), H₂O(ideal gas) 3-31-79.

Water (H₂O) H_2O_1(l)

Water (H₂O)   IDEAL GAS M_r = 18.01528   H₂O₁(g)

$\Delta_a H°(0\ K) = 917.769 \pm 0.109\ \text{kJ·mol}^{-1}$
$S°(298.15\ K) = 188.834 \pm 0.042\ \text{J·K}^{-1}\text{·mol}^{-1}$

$\Delta_f H°(0\ K) = -238.921 \pm 0.042\ \text{kJ·mol}^{-1}$
$\Delta_f H°(298.15\ K) = -241.826 \pm 0.042\ \text{kJ·mol}^{-1}$

Vibrational Frequencies and Degeneracies[a]
ν, cm⁻¹
3651.1(1)
1594.7(1)
3755.9(1)

Point Group: C_{2v} $\sigma = 2$
Rotational Constants[a]: $A_0 = 27.8847$ cm⁻¹ $B_0 = 14.5118$ cm⁻¹ $C_0 = 9.2806$ cm⁻¹
[a]See Wooley[4] for detailed molecular constants on which this table is based.

Enthalpy of Formation
The adopted value of $\Delta_f H°(298.15\ K)$ is that recommended by CODATA[1] and was calculated by CODATA from the heat of formation of liquid water at 298.15 K using vaporization data given by Keenan et al.[2] The enthalpy of atomization, $\Delta_a H°(0\ K) = 219.352 \pm 0.026$ kcal·mol⁻¹, is calculated using auxiliary JANAF data.[3]

Heat Capacity and Entropy
The adopted heat capacity and entropy data below 2000 K, which are for water with the natural isotopic abundance, are taken from recent calculations by Wooley.[4] Wooley has done detailed calculations on the thermodynamic functions of light isotopic water ($^1H_2{}^{16}O$) and then corrected those to functions appropriate for water of natural isotopic abundance. Below 240 K, his calculation was a direct summation over rotational levels of the group vibrational state, with small additions above 130 K for the $\nu_2=1$ vibrational level. Above 240 K, individual vibrational partition functions were summed to obtain the total partition function. During this summation the molecule was treated as a rigid rotator with modified corrections of Stripp-Kirkwood and centrifugal effect types, guided by the behavior found for the vibrational ground state. Details are given by Woolley.[4]

Between 2000 and 5000 K we adopt $C_p°$ data calculated by Friedman and Haar[5] for light isotopic water, after a small correction. Our correction consists of adding 0.021 cal·K⁻¹·mol⁻¹ to Friedman and Haar's $C_p°$ data. This correction arises from the constant difference of 0.021 ± 0.001 cal·K⁻¹·mol⁻¹ between Woolley's $C_p°$ data (natural abundance) and Friedman and Haar's $C_p°$ data (light isotopic water) in the temperature range 1300–2000 K. Above 5000 K, we have linearly extrapolated Friedman and Haar's corrected $C_p°$ data.

Below 2000 K there is good agreement among thermodynamic functions given by Woolley,[4] Friedman and Haar[5] and Glushko et al.[6] Above 2000 K the $C_p°$ data from references[5] and[6] begin to deviate significantly; at 4000 and 6000 K the differences $[C_p°^6-C_p°^5]$ are 0.57 and 1.07 cal·K⁻¹·mol⁻¹, respectively. Woolley is working on extending his calculations to higher temperature[7] and his initial results[7] yield $C_p°$ values slightly higher than[5] but not nearly so high as.[6]

Values of $S°(298.15\ K)$ and $H°(298.15\ K)-H°(0\ K)$ in the present table are in excellent agreement with CODATA values[1] of 45.106 ± 0.01 cal·K⁻¹·mol⁻¹ and 2.368 ± 0.002 kcal·mol⁻¹, respectively.

References
[1]ICSU–CODATA Task Group, J. Chem. Thermodyn. 4, 331 (1972); also refer to, CODATA Bulletin #17, "CODATA Recommended Key Values for Thermodynamics– 1975," (1976).
[2]J. H. Keenan, F. G. Keyes, P. G. Hill and J. G. Moore, "Steam Tables," Wiley, New York, (1969).
[3]JANAF Thermochemical Tables: H(g), O(g), 3-31-77.
[4]H. W. Woolley, U. S. Nat. Bur. Stand., paper presented at the 9th International Conference on the Properties of Steam, Munich, Sept. 10–14, (1979).
[5]A. S. Friedman and L. Haar, J. Chem. Phys. 22, 2051 (1954).
[6]V. P. Glushko, L. V. Gurvich et al., "Thermodynamic Properties of Individual Substances," Third edition, Volume 1, Book 1, Nauka, Moscow, (1978).
[7]H. W. Woolley, U. S. Nat. Bur. Stand., personal communication, (August 1980).

Water (H₂O)   Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa   H₂O₁(g)

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	J·K⁻¹·mol⁻¹			kJ·mol⁻¹			
0	0.	0.	INFINITE	-9.904	-238.921	-238.921	INFINITE
100	33.299	152.388	218.534	-6.615	-240.083	-236.584	123.579
200	33.349	175.485	191.896	-3.282	-240.900	-232.766	60.792
298.15	33.590	188.834	188.834	0.	-241.826	-228.582	40.047
300	33.596	189.042	188.835	0.062	-241.844	-228.500	39.785
400	34.262	198.788	190.159	3.452	-242.846	-223.901	29.238
500	35.226	206.534	192.685	6.925	-243.826	-219.051	22.884
600	36.325	213.052	195.550	10.501	-244.758	-214.007	18.631
700	37.495	218.739	198.465	14.192	-245.632	-208.812	15.582
800	38.721	223.825	201.322	18.002	-246.443	-203.496	13.287
900	39.987	228.459	204.084	21.938	-247.185	-198.083	11.496
1000	41.268	232.738	206.738	26.000	-247.857	-192.590	10.060
1100	42.536	236.731	209.285	30.191	-248.460	-187.033	8.881
1200	43.768	240.485	211.730	34.506	-248.997	-181.425	7.897
1300	44.945	244.035	214.080	38.942	-249.473	-175.774	7.063
1400	46.054	247.407	216.341	43.493	-249.894	-170.089	6.346
1500	47.090	250.620	218.520	48.151	-250.265	-164.376	5.724
1600	48.050	253.690	220.623	52.908	-250.592	-158.639	5.179
1700	48.935	256.630	222.655	57.758	-250.881	-152.883	4.698
1800	49.749	259.451	224.621	62.693	-251.138	-147.111	4.269
1900	50.496	262.161	226.526	67.706	-251.368	-141.325	3.885
2000	51.180	264.769	228.374	72.790	-251.575	-135.528	3.540
2100	51.823	267.282	230.167	77.941	-251.762	-129.721	3.227
2200	52.408	269.706	231.909	83.153	-251.934	-123.905	2.942
2300	52.947	272.048	233.604	88.421	-252.092	-118.082	2.682
2400	53.444	274.312	235.253	93.741	-252.239	-112.252	2.443
2500	53.904	276.503	236.860	99.108	-252.379	-106.416	2.223
2600	54.329	278.625	238.425	104.520	-252.513	-100.575	2.021
2700	54.723	280.683	239.952	109.973	-252.643	-94.729	1.833
2800	55.089	282.680	241.443	115.464	-252.771	-88.878	1.658
2900	55.430	284.619	242.899	120.990	-252.897	-83.023	1.495
3000	55.748	286.504	244.321	126.549	-253.024	-77.163	1.344
3100	56.044	288.337	245.711	132.139	-253.152	-71.298	1.201
3200	56.323	290.120	247.071	137.757	-253.282	-65.430	1.068
3300	56.583	291.858	248.402	143.403	-253.416	-59.558	0.943
3400	56.828	293.550	249.705	149.073	-253.553	-53.681	0.825
3500	57.058	295.201	250.982	154.768	-253.696	-47.801	0.713
3600	57.276	296.813	252.233	160.485	-253.844	-41.916	0.608
3700	57.480	298.384	253.459	166.222	-253.997	-36.027	0.509
3800	57.675	299.919	254.661	171.980	-254.158	-30.133	0.414
3900	57.859	301.420	255.841	177.757	-254.326	-24.236	0.325
4000	58.033	302.887	256.999	183.552	-254.501	-18.334	0.239
4100	58.199	304.322	258.136	189.363	-254.684	-12.427	0.158
4200	58.357	305.726	259.252	195.191	-254.876	-6.516	0.081
4300	58.507	307.101	260.349	201.034	-255.078	-0.600	0.007
4400	58.650	308.448	261.427	206.892	-255.288	5.320	-0.063
4500	58.787	309.767	262.486	212.764	-255.508	11.245	-0.131
4600	58.918	311.061	263.528	218.650	-255.738	17.175	-0.195
4700	59.044	312.329	264.553	224.548	-255.978	23.111	-0.257
4800	59.164	313.574	265.562	230.458	-256.229	29.052	-0.316
4900	59.275	314.795	266.554	236.380	-256.491	34.998	-0.373
5000	59.390	315.993	267.531	242.313	-256.763	40.949	-0.428
5100	59.509	317.171	268.493	248.258	-257.046	46.906	-0.480
5200	59.628	318.327	269.440	254.215	-257.338	52.869	-0.531
5300	59.746	319.464	270.373	260.184	-257.639	58.838	-0.580
5400	59.864	320.582	271.293	266.164	-257.950	64.811	-0.627
5500	59.982	321.682	272.199	272.157	-258.268	70.791	-0.672
5600	60.100	322.764	273.092	278.161	-258.595	76.777	-0.716
5700	60.218	323.828	273.973	284.177	-258.930	82.769	-0.758
5800	60.335	324.877	274.841	290.204	-259.272	88.767	-0.799
5900	60.453	325.909	275.698	296.244	-259.621	94.770	-0.839
6000	60.571	326.926	276.544	302.295	-259.977	100.780	-0.877

PREVIOUS: March 1961 (1 atm)   CURRENT: March 1979 (1 bar)