AMMONIA (NH₃)

AMMONIA (NH$_3$)

(IDEAL GAS) GFW=17.0304

H$_3$N

T, K	Cp°	S°	-(G°-H°₂₉₈)/T	H°-H°₂₉₈	ΔHf°	ΔGf°	Log Kp
		gibbs/mol			kcal/mol		
0	0.000	0.000	INFINITE	-2.401	-9.299	-9.299	INFINITE
100	7.955	37.221	53.322	-1.810	-9.930	-8.137	17.782
200	8.068	42.753	46.810	-0.811	-10.445	-6.143	6.712
298	8.521	46.048	46.048	0.000	-10.970	-3.920	2.873
300	8.533	46.101	46.048	0.016	-10.980	-3.876	2.824
400	9.253	48.650	46.391	0.904	-11.482	-1.430	0.781
500	10.050	50.801	47.063	1.869	-11.917	1.134	-0.496
600	10.825	52.702	47.847	2.913	-12.279	3.779	-1.377
700	11.557	54.426	48.666	4.032	-12.576	6.480	-2.023
800	12.245	56.015	49.486	5.223	-12.816	9.219	-2.518
900	12.894	57.495	50.295	6.480	-13.005	11.985	-2.910
1000	13.502	58.885	51.085	7.800	-13.149	14.770	-3.228
1100	14.068	60.199	51.854	9.179	-13.253	17.567	-3.490
1200	14.591	61.446	52.602	10.612	-13.324	20.373	-3.710
1300	15.071	62.633	53.329	12.096	-13.365	23.182	-3.897
1400	15.510	63.766	54.034	13.625	-13.380	25.995	-4.058
1500	15.909	64.850	54.719	15.197	-13.374	28.807	-4.197
1600	16.271	65.889	55.385	16.806	-13.348	31.618	-4.319
1700	16.599	66.885	56.032	18.450	-13.306	34.427	-4.426
1800	16.896	67.842	56.662	20.125	-13.251	37.233	-4.521
1900	17.165	68.763	57.275	21.828	-13.183	40.037	-4.605
2000	17.408	69.650	57.872	23.557	-13.106	42.836	-4.681
2100	17.627	70.505	58.453	25.309	-13.019	45.631	-4.749
2200	17.825	71.329	59.020	27.081	-12.927	48.421	-4.810
2300	18.004	72.126	59.572	28.873	-12.828	51.208	-4.866
2400	18.166	72.896	60.111	30.682	-12.724	53.990	-4.916
2500	18.314	73.640	60.638	32.506	-12.616	56.768	-4.963
2600	18.445	74.361	61.152	34.344	-12.507	59.541	-5.005
2700	18.564	75.059	61.654	36.194	-12.394	62.311	-5.044
2800	18.674	75.737	62.145	38.056	-12.282	65.074	-5.079
2900	18.769	76.394	62.625	39.929	-12.168	67.835	-5.112
3000	18.858	77.031	63.095	41.810	-12.053	70.593	-5.143
3100	18.936	77.651	63.554	43.700	-11.940	73.346	-5.171
3200	19.006	78.253	64.004	45.597	-11.829	76.094	-5.197
3300	19.069	78.839	64.445	47.501	-11.718	78.841	-5.221
3400	19.123	79.409	64.877	49.411	-11.610	81.583	-5.244
3500	19.172	79.964	65.300	51.325	-11.505	84.323	-5.265
3600	19.216	80.505	65.715	53.245	-11.403	87.059	-5.285
3700	19.252	81.032	66.122	55.168	-11.305	89.793	-5.304
3800	19.284	81.546	66.521	57.095	-11.211	92.524	-5.321
3900	19.310	82.047	66.913	59.025	-11.122	95.252	-5.338
4000	19.331	82.536	67.297	60.957	-11.038	97.978	-5.353
4100	19.349	83.014	67.675	62.891	-10.958	100.703	-5.368
4200	19.361	83.480	68.045	64.826	-10.884	103.426	-5.382
4300	19.371	83.936	68.410	66.763	-10.816	106.146	-5.395
4400	19.375	84.381	68.768	68.700	-10.754	108.867	-5.407
4500	19.377	84.817	69.119	70.638	-10.699	111.583	-5.419
4600	19.373	85.243	69.465	72.576	-10.650	114.301	-5.430
4700	19.367	85.659	69.805	74.513	-10.609	117.016	-5.441
4800	19.357	86.067	70.140	76.449	-10.574	119.732	-5.451
4900	19.343	86.466	70.469	78.384	-10.547	122.446	-5.461
5000	19.325	86.856	70.793	80.317	-10.527	125.161	-5.471
5100	19.300	87.239	71.112	82.248	-10.516	127.873	-5.480
5200	19.300	87.614	71.425	84.178	-10.511	130.587	-5.488
5300	19.300	87.981	71.734	86.108	-10.511	133.301	-5.497
5400	19.300	88.342	72.039	88.038	-10.518	136.014	-5.505
5500	19.300	88.696	72.338	89.968	-10.528	138.728	-5.512
5600	19.300	89.044	72.633	91.898	-10.542	141.443	-5.520
5700	19.300	89.386	72.924	93.828	-10.562	144.156	-5.527
5800	19.300	89.721	73.211	95.758	-10.585	146.871	-5.534
5900	19.300	90.051	73.494	97.688	-10.612	149.586	-5.541
6000	19.300	90.376	73.772	99.618	-10.644	152.300	-5.547

Dec. 31, 1960; Mar. 31, 1961; Sept. 30, 1965;
July 31, 1972 (NBS); June 30, 1977

AMMONIA (NH$_3$)   (IDEAL GAS)   GFW = 17.0304

H$_3$N

Point Group C$_{3v}$
S°$_{298.15}$ = 46.048 ± 0.006 gibbs/mol
Ground State Quantum Weight = 1

ΔHf°$_0$ = -9.30 ± 0.1 kcal/mol
ΔHf°$_{298.15}$ = -10.97 ± 0.1 kcal/mol

Vibrational Frequencies and Degeneracies

ω, cm^{-1}	ω, cm^{-1}	ω, cm^{-1}	ω, cm^{-1}
3506 (1)	1022 (1)	3577 (2)	1691 (2)

Bond Length: N-H = 1.0124 Å   σ(external) = 3
Bond Angle: 106.67°   σ(internal) = 2
Product of the Moments of Inertia: $I_A I_B I_C$ = 3.4824 x 10^{-119} g^{3}cm^6

Heat of Formation

Second and third law analyses of equilibrium data for the reaction $1/2N_2(g)+3/2H_2(g) = NH_3(g)$ cited in the previous JANAF evaluation (1) plus more recent work of Schulz and Schaefer (6) were made using the revised thermal functions for NH$_3$(g). All of the previously cited work in reaction calorimetry plus the early work of Berthelot (7, 8) and Thomsen (9) were reevaluated. No significant differences in the third law calculations of the equilibrium data or in the corrections to the flow calorimetry data of Haber and Tamaru (12) and Wittig and Schmatz (13) were found. Thus, the 0.1 kcal discrepancy between the results of the equilibrium and reaction calorimetry measurements remains unresolved. The previous JANAF selection (1) for ΔHf°$_{298}$ of NH$_3$(g) was adopted. A recent evaluation (14) which includes new indirect calorimetry (unpublished) further confirms this selection.

Source	Method	ΔHf°$_{298}$ kcal/mol	ΔHf°$_{298}$ kcal/mol*	ΔS°$_{298}$(obs.-calc.)* (e.u.)
Larson, Dodge (2, 1923)	Kp(4) from Kp(10-1,000 atm, 600-800 K)	-10.88	-10.70±0.11	+0.24±0.15^a
Haber et al. (3, 1915)	Kp(4) from Kp(30 atm, 800-1200 K)	-10.86	-10.88±0.15	-0.02±0.15^b
Haber, Maschke (5, 1915)	Kp(1 atm, 900-1400 K)	-10.85	-10.62±0.22	0.20±0.19^c
Schulz, Schaefer (6, 1966)	Kp(1 atm, 567-673 K)	-10.87	-10.78±0.20	0.14±0.3^d
Berthelot (7, 1880)	Indirect; Reaction of Br$_2$(aq) and NH$_3$(aq)	-11.4		
Berthelot (8, 1880)	Indirect; Reaction of O$_2$(g) with NH$_3$(g)	-12.1		
Thomsen (9, 1882)	Indirect; Reaction of O$_2$(g) with NH$_3$(g)	-11.9		
Becker, Roth (10, 1934)	Indirect; Heat of combustion oxalates	-11.00±0.15		
Haber et al. (11, 1915)	Flow calorimetry at 298 K	-11.10±0.05		
Haber, Tamaru (12, 1915)	Flow calorimetry (739-932 K)	-10.97±0.008		
Wittig, Schmatz (13, 1959)	Flow calorimetry at 832 K	-10.99±0.05		

*Second law analysis assuming ΔCp (gibbs/mol) equals (a) -2.672+0.00591(T-700), (b) -1.236+0.00404(T-1000), (c) -0.855+0.00305(T-1100), (d) -3.287+0.00651(T-600).

Heat Capacity and Entropy

The thermodynamic functions differ from those of the 1965 JANAF table (1) in being taken directly from the later and more complete work of Haar (15). Haar treated in detail the contribution of the highly anharmonic out-of-plane vibrational mode, including its large coupling with rotation and its coupling with the other vibrational modes. Haar's values of C$_p^\circ$ pass through a shallow maximum between 4000 and 5000 K; they were extrapolated from 5000 to 6000 K by assuming a constant value (19.300 gibbs/mol). A summary of Haar's estimated uncertainties and of the differences of the 1965 table from the present table (in gibbs/mol) is as follows:

T, K	Uncertainties (Haar, 15)		1965 Table minus This Table	
	Cp°	S°	Cp°	S°
1000	0.006	0.006	-0.034	-0.033
3000	0.10	0.06	+0.142	-0.122
5000	0.6	0.4	+1.775	+0.265

The National Bureau of Standards prepared this table (16) by critical analysis of data existing in 1972. Using the results of Haar (15) and ΔHf° selected by NBS (16), we recalculate the table in terms of R=1.987192 cal/(mol K) (17) and current JANAF reference states for the elements.

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H$_3$N