

Manganese (Mn)

A₁ = 54.9380 Manganese (Mn)

REFERENCE STATE

- 0 to 980 K crystal, alpha
- 980 to 1360 K crystal, beta
- 1360 to 1410 K crystal, gamma
- 1410 to 1517 K crystal, delta
- 1517 to 2335 K liquid
- 2335 to 6000 K ideal gas, monatomic

Refer to the individual tables for details.

Mn₁(ref)

T/K	Enthalpy Reference Temperature = T ₁ = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K ₁
	C _p ^o	S° - [C _p ^o - HF(T ₁)]/T	H° - H°(T ₁)	Δ _f H°	
		J·K ⁻¹ ·mol ⁻¹	kJ·mol ⁻¹		
0	0.	0.	INFINITE	0.	0.
100	14.723	8.875	52.876	0.	0.
200	23.054	22.133	34.325	0.	0.
298.15	26.299	32.010	32.010	0.	0.
300	26.347	32.173	32.010	0.049	0.049
400	28.527	40.066	33.072	2.798	0.
500	30.292	46.696	35.152	5.772	0.
600	31.899	52.362	37.589	8.882	0.
700	33.426	57.395	40.030	12.149	0.
800	34.915	61.956	42.498	15.566	0.
900	36.384	66.153	44.896	19.151	0.
980.000	37.545	69.300	46.761	22.088	ALPHA <--> BETA
980.000	37.572	71.572	46.761	24.314	TRANSITION
1000	37.698	72.332	47.265	25.067	0.
1100	38.116	75.945	49.710	28.858	0.
1200	38.535	79.279	52.037	32.690	0.
1300	38.953	82.380	54.253	36.565	0.
1361.000	39.204	84.172	55.554	38.948	BETA <--> GAMMA
1361.000	43.095	85.731	55.554	41.070	TRANSITION
1400	43.430	86.953	56.412	42.757	0.
1412.000	43.514	87.324	56.673	43.279	GAMMA <--> DELTA
1412.000	45.229	88.655	56.673	45.158	TRANSITION
1500	45.982	91.413	58.631	49.173	0.
1519.000	46.108	91.993	59.045	50.048	DELTA <--> LIQUID
1519.000	46.024	99.931	59.045	62.106	TRANSITION
1600	46.024	102.322	61.176	65.834	0.
1700	46.024	105.112	63.679	70.436	0.
1800	46.024	107.743	66.055	75.039	0.
1900	46.024	110.231	68.315	79.641	0.
2000	46.024	112.592	70.470	84.244	0.
2100	46.024	114.837	72.530	88.846	0.
2200	46.024	116.978	74.502	93.448	0.
2300	46.024	119.024	76.393	98.051	0.
2334.526	46.024	119.710	77.029	99.640	LIQUID <--> IDEAL GAS
2334.526	20.951	216.509	77.029	325.620	FUGACITY = 1 bar
2400	20.997	217.089	80.842	326.993	0.
2500	21.085	217.948	86.309	329.097	0.
2600	21.198	218.777	91.388	331.211	0.
2700	21.341	219.580	96.121	333.338	0.
2800	21.515	220.359	100.545	335.480	0.
2900	21.726	221.118	104.689	337.642	0.
3000	21.976	221.858	108.583	339.827	0.
3100	22.269	222.583	112.248	342.039	0.
3200	22.606	223.296	115.708	344.282	0.
3300	22.990	223.997	118.978	346.561	0.
3400	23.424	224.690	122.077	348.882	0.
3500	23.909	225.376	125.019	351.248	0.
3600	24.445	226.056	127.816	353.665	0.
3700	25.034	226.734	130.480	356.139	0.
3800	25.675	227.410	133.022	358.674	0.
3900	26.370	228.086	135.451	361.275	0.
4000	27.118	228.763	137.776	363.949	0.
4200	28.772	230.125	142.141	369.535	0.
4400	30.633	231.506	146.171	375.472	0.
4600	32.668	232.907	149.912	381.777	0.
4800	34.798	234.340	153.399	388.514	0.
5000	37.153	235.808	156.666	395.707	0.
5200	39.664	237.313	159.739	403.386	0.
5400	42.327	238.860	162.641	411.582	0.
5600	45.144	240.321	165.382	419.658	0.
5800	48.114	241.887	167.993	428.580	0.
6000	47.832	243.472	170.483	437.936	0.

PREVIOUS:

CURRENT: September 1967 (1 bar)

Manganese (Mn)

Mn₁(ref)

CRYSTAL (α , β , γ , δ)

Manganese (Mn)

Manganese (Mn)

Mn₁(cr)

$S^\circ(298.15\text{ K}) = 32.01 \pm 0.08\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
 $T_m(\alpha \rightarrow \beta) = 980 \pm 20\text{ K}$
 $T_m(\beta \rightarrow \gamma) = 1361 \pm 10\text{ K}$
 $T_m(\gamma \rightarrow \delta) = 1412 \pm 5\text{ K}$
 $T_m(\delta \rightarrow l) = 1519 \pm 5\text{ K}$

Enthalpy of Formation

Zero by definition.

Heat Capacity and Entropy

A thorough re examination of the manganese thermal functions is in process. Temporarily, the recommendations of Hultgren *et al.*¹ are adopted. These results are based on the heat capacity studies of Scurlock and Stevens (0.3–1.0 K),² Gaumer (0.64–3 K),³ Guthrie *et al.* (1.7–4.2 K),⁴ Booth *et al.* (12–20 K),⁵ Kelley (52–298 K),⁶ and Shomate (373–1436 K).⁷ As Hultgren *et al.*¹ states, the study of Naylor was chosen because it covers all forms of Mn in a self consistent manner. It is not stated why Hultgren, *et al.*¹ altered Naylor's equations,⁸ which appear more appropriate than the current values.

Phase and Fusion Data

As we are temporarily adopting the analysis of Hultgren, *et al.*¹ we rely on his analysis of the transition and fusion temperatures. Ten studies are analyzed by Hultgren *et al.*¹ The temperatures were adjusted to IPTS–68.

Sublimation Data

Refer to the ideal gas table for details.

References

- ¹R. Hultgren, P. D. Desai, *et al.*, "Selected Values of the Thermodynamic Properties of the Elements," American Society for Metals, Metals Park, Ohio, (1973).
- ²R. G. Scurlock and W. N. R. Stevens, *Proc. Phys. Soc.* **86**, 331 (1965).
- ³R. E. Gaumer, Ohio State University, Ph. D. Thesis, (1959).
- ⁴G. L. Guthrie, S. A. Friedburg, and J. E. Goldman, *Phys. Rev.* **139**, 1200 (1965).
- ⁵G. L. Booth, F. E. Hoare and B. T. Murphy, *Proc. Phys. Soc.* **68**, 830 (1955).
- ⁶K. K. Kelley, *J. Am. Chem. Soc.* **61**, 203 (1939).
- ⁷C. H. Shomate, U. S. Bur. Mines Tech. Paper 686, pp. 2–11 (1946).
- ⁸B. F. Naylor, *J. Chem. Phys.* **13**, 329 (1945).

T/K	C _p ^o	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p ^o = 0.1 MPa		log K _r
		J·K ⁻¹ ·mol ⁻¹	S ^o - [C _p ^o - HR(T _r)]/T	H ^o - H ^o (T _r)	Δ _r G ^o	
0	0	INFINITE	0	-4594	0	0
100	14.723	8.875	52.876	-4.400	0	0
200	23.054	22.133	34.325	-2.438	0	0
250	24.948	27.493	32.436	-1.236	0	0
298.15	26.299	32.010	32.010	0	0	0
300	26.347	32.173	32.010	0.049	0	0
350	27.516	36.325	32.336	1.396	0	0
400	28.527	40.066	33.072	2.798	0	0
450	30.020	43.524	34.043	4.266	0	0
500	30.292	46.696	35.152	5.772	0	0
600	31.899	52.362	37.559	8.882	0	0
700	33.426	57.395	40.039	12.149	0	0
800	34.915	61.956	42.498	15.566	0	0
900	36.384	66.153	44.896	19.131	0	0
980.000	37.545	69.300	46.761	22.088	0	0
980.000	37.572	71.572	46.761	24.314	ALPHA <--> BETA TRANSITION	0
1000	37.698	72.332	47.265	25.067	0	0
1100	38.116	75.945	49.710	28.858	0	0
1200	38.535	79.279	52.037	32.690	0	0
1300	38.953	82.380	54.255	36.563	0	0
1361.000	39.204	84.172	55.554	38.948	BETA <--> GAMMA TRANSITION	0
1361.000	43.095	85.731	55.554	41.070	0	0
1400	43.430	86.953	56.412	42.757	0	0
1412.000	43.514	87.324	56.673	43.279	GAMMA <--> DELTA TRANSITION	0
1412.000	45.229	88.655	56.673	45.158	0	0
1500	45.982	91.413	58.631	49.173	0	0
1519.000	46.108	91.993	59.045	50.048	DELTA <--> LIQUID	0
1600	46.803	94.406	60.774	53.811	-12.023	0.642
1700	47.624	97.268	62.837	58.532	-11.904	1.431
1800	48.476	100.913	64.827	63.336	-11.703	2.210
1900	49.267	102.653	66.749	68.221	-11.420	2.975

PREVIOUS:

CURRENT: September 1967

Manganese (Mn)

Mn₁(cr)

Manganese (Mn) Mn₁(l)

LIQUID

$A_1 = 54.9380$ Manganese (Mn) $A_2 = 54.9380$ Manganese (Mn)

$S^\circ(298.15\text{ K}) = [43.4991\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}]$
 $T_{\text{lim}} = 1519 \pm 5\text{ K}$
 $\Delta_f H^\circ(298.15\text{ K}) = [16.289]\text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta_{\text{vap}} H^\circ = 12.058 \pm 1.0\text{ kJ}\cdot\text{mol}^{-1}$

Enthalpy of Formation
 The enthalpy of formation of Mn(l), $\Delta_f H^\circ(298.15\text{ K})$ is calculated from that of the crystal by adding $\Delta_{\text{vap}} H^\circ$ and the difference in enthalpy, $H^\circ(1519\text{ K}) - H^\circ(298.15\text{ K})$, between the crystal and liquid.

Heat Capacity and Entropy
 Hultgren¹ adopted $C_p^\circ(l) = 11.0\text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ based on the recommendation of Kelly.² A glass transition temperature is assumed at 1125 K, below which the heat capacity values of $\alpha\text{-Mn}(cr)$ are adopted, a re-examination of Mn(l) is in progress. The entropy at 298.15 K is calculated in a manner analogous to that used for the enthalpy of formation.

Vaporization Data
 $T_{\text{vap}}(1\text{ bar})$ is calculated as the temperature at which $\Delta_f G^\circ = 0$ for the process $\text{Mn}(l) = \text{Mn}(g)$. $\Delta_{\text{vap}} H^\circ$ is calculated as the difference in the enthalpies of formation of Mn(l) and Mn(g) at T_{vap} .

References
¹R. Hultgren, P. D. Desai, *et al.*, "Selected Values of the Thermodynamic Properties of the Elements," American Society for Metals, Metals Park, Ohio, (1973).
²K. K. Kelley, U. S. Bur. Mines Bull. 584, 232 pp. (1960).

T/K	C_p°	S°	$-[G^\circ - H^\circ(T)]/T$	$H^\circ - H^\circ(T)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K _r
0							
100							
200							
250							
298.15	26.299	43.499	43.499	0.	16.289	12.863	-2.254
300	26.347	43.662	43.500	0.049	16.289	12.842	-2.236
350	27.516	47.814	43.825	1.396	16.289	12.267	-1.831
400	28.527	51.555	44.261	2.798	16.289	11.693	-1.527
450	30.020	55.013	45.353	4.266	16.289	11.118	-1.291
500	30.292	58.185	46.642	5.772	16.289	10.544	-1.102
600	31.899	63.852	49.048	8.882	16.289	9.395	-0.818
700	33.426	68.884	51.529	12.149	16.289	8.246	-0.615
800	34.915	73.445	53.988	15.566	16.289	7.097	-0.463
900	36.384	77.643	56.386	19.131	16.289	5.948	-0.345
1000	37.834	81.551	58.709	22.842	14.064	4.845	-0.253
1100	39.275	85.225	60.954	26.698	14.129	3.921	-0.186
1125.000	39.634	86.111	61.503	27.684	GLASS <--> LIQUID		
1125.000	46.024	86.111	61.503	27.684	TRANSITION		
1200	46.024	89.082	63.135	31.136	14.734	2.971	-0.129
1300	46.024	92.766	65.275	35.738	15.462	1.961	-0.079
1400	46.024	96.176	67.362	40.341	13.872	0.960	-0.036
1500	46.024	99.352	69.390	44.943	12.059	0.151	-0.005
1519.000	46.024	99.931	69.768	45.817	DELTA <--> LIQUID		
1600	46.024	102.322	71.356	49.545	0.	0.	0.
1700	46.024	105.112	73.280	54.148	0.	0.	0.
1800	46.024	107.743	75.104	58.750	0.	0.	0.
1900	46.024	110.231	76.888	63.353	0.	0.	0.
2000	46.024	112.592	78.614	67.955	0.	0.	0.
2100	46.024	114.837	80.286	72.557	0.	0.	0.
2200	46.024	116.978	81.906	77.160	0.	0.	0.
2300	46.024	119.024	83.476	81.762	0.	0.	0.
2334.526	46.024	119.710	84.006	83.351	FUGACITY = 1 bar		
2400	46.024	120.983	84.998	86.365	-224.340	6.315	-0.137
2500	46.024	122.862	86.475	90.967	-221.841	15.874	-0.332
2600	46.024	124.667	87.909	95.569	-219.353	25.334	-0.509
2700	46.024	126.404	89.303	100.172	-216.877	34.698	-0.671
2800	46.024	128.078	90.658	104.774	-214.417	43.970	-0.820
2900	46.024	129.693	91.977	109.377	-211.977	53.155	-0.957
3000	46.024	131.253	93.260	113.979	-209.559	62.256	-1.084

PREVIOUS: CURRENT: September 1967

Manganese (Mn) Mn₁(l)

CRYSTAL(α , β , γ , δ)-LIQUID

0 to 980 K crystal, alpha
 980 to 1361 K crystal, beta
 1361 to 1412 K crystal, gamma
 1412 to 1519 K crystal, delta
 above 1519 K liquid

Refer to the individual tables for details.

Manganese (Mn)

Manganese (Mn)

Mn₁(cr,l)

Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p° = 0.1 MPa				
T/K	C _p ^o	S° - [G° - H°(T _r)]/T	H° - H°(T _r) / kJ·mol ⁻¹	$\Delta_f H^\circ$	ΔG°	log K _f
0	0.	INFINITE	0.	0.	0.	0.
100	14.723	8.875	52.876	-4.994	0.	0.
200	21.054	22.133	34.325	-4.400	0.	0.
250	24.948	27.493	32.436	-2.438	0.	0.
298.15	26.299	32.010	32.010	-1.236	0.	0.
300	26.347	32.173	32.010	0.	0.	0.
350	27.516	36.323	32.336	0.049	0.	0.
400	28.577	40.066	33.072	1.306	0.	0.
450	30.020	43.574	34.045	2.708	0.	0.
500	30.292	46.696	35.152	4.266	0.	0.
600	31.899	52.362	37.559	5.772	0.	0.
700	33.426	57.395	40.039	8.882	0.	0.
800	34.915	61.956	42.498	12.149	0.	0.
900	36.384	66.153	44.896	15.566	0.	0.
980.000	37.545	69.300	46.761	19.131	0.	0.
980.000	37.572	71.572	46.761	22.088	ALPHA \leftrightarrow BETA TRANSITION	0.
1000	37.698	72.332	47.265	24.314	0.	0.
1100	38.116	75.945	49.710	25.067	0.	0.
1200	38.535	79.279	52.037	28.838	0.	0.
1300	38.953	82.380	54.253	32.690	0.	0.
1361.000	39.204	84.172	55.554	36.565	BETA \leftrightarrow GAMMA TRANSITION	0.
1361.000	43.095	85.731	55.554	38.948	0.	0.
1400	43.430	86.953	56.412	41.070	0.	0.
1412.000	43.514	87.324	56.673	42.757	0.	0.
1412.000	45.229	88.655	56.673	43.279	GAMMA \leftrightarrow DELTA TRANSITION	0.
1500	45.982	91.413	58.631	45.158	0.	0.
1519.000	46.108	91.983	59.045	49.173	0.	0.
1519.000	46.024	99.931	59.045	50.048	DELTA \leftrightarrow LIQUID TRANSITION	0.
1600	46.024	102.322	61.176	62.106	0.	0.
1700	46.024	105.112	63.679	65.834	0.	0.
1800	46.024	107.743	66.055	70.436	0.	0.
1900	46.024	110.231	68.315	75.039	0.	0.
2000	46.024	112.592	70.470	79.641	0.	0.
2100	46.024	114.837	72.530	84.244	0.	0.
2200	46.024	116.978	74.502	88.846	0.	0.
2300	46.024	119.024	76.393	93.448	0.	0.
2334.526	46.024	119.710	77.029	98.051	0.	0.
2400	46.024	120.983	78.211	99.640	FUGACITY = 1 bar	0.
2500	46.024	122.862	79.960	102.653	-224.340	6.315
2600	46.024	124.667	81.645	107.256	-221.841	15.874
2700	46.024	126.404	83.270	111.858	-219.353	25.334
2800	46.024	128.078	84.841	116.460	-216.877	34.698
2900	46.024	129.693	86.360	121.063	-214.417	43.970
3000	46.024	131.253	87.830	125.665	-211.977	53.155
				130.268	-209.559	62.256
						-1.084

PREVIOUS:

CURRENT September 1967

Manganese (Mn)

Mn₁(cr,l)

Manganese (Mn)

IDEAL GAS

Manganese (Mn)

Mn₁(g)

IP (Mn, g) = 59981 ± 1 cm⁻¹
 S°(298.15 K) = 173.716 J·K⁻¹·mol⁻¹

ΔH^o(0 K) = 282.1 ± 4.2 kJ·mol⁻¹
 ΔH^o = (298.15 K) = 283.3 ± 4.2 kJ·mol⁻¹

Electronic Levels and Quantum Weights	g _e
State	ε _e , cm ⁻¹
⁶ S _{5/2}	0.00
⁶ D _{5/2}	17052.29
⁶ D _{7/2}	17282.00
⁶ D _{3/2}	17451.52
⁶ D _{1/2}	17568.48
⁶ D _{1/2}	17637.15

Enthalpy of Formation

The value adopted for the enthalpy of formation of Mn(g), ΔH^o(298.15 K) = 283.3 ± 4.2 kJ·mol⁻¹, is that recommended by Hultgren *et al.*¹ This value is a weighted mean of sublimation and vaporization studies. The studies are Bogatyrev and Golubisov (1043–1168 K),² Pratt and Spencer (1248–1620 K),³ Wiedemeier (1269–1448 K),⁴ Butler *et al.* (1075–1335 K),⁵ Woolf, *et al.* (1523–1823 K),⁶ McCabe and Hudson (1075–1235 K),⁷ and Baur and Brunner (1587–1987 K).⁸
 A reanalysis of the vapor pressure data is in progress.

Heat Capacity and Entropy

The information on electronic energy levels and quantum weights, given by Corliss and Sugar,⁹ is incomplete because many theoretically predicted levels have not been observed. Although we have listed only a few of the lowest lying levels for Mn(g), all levels listed by Corliss and Sugar,⁹ as well as estimated levels, are used in the calculation. The observed levels are too numerous to list completely. The calculations indicate that for Mn(g), the thermodynamic functions are independent of the estimated missing levels (for n = 4–8), the cut-off procedure, and the inclusion of n > 9 levels up to 4000 K; the Gibbs energy function showing no significant variations at this temperature. The reported uncertainty in S°(298.15 K) is due to uncertainties in the relative ionic mass, and the fundamental constants. Extension of these calculations above 6000 K may require consideration of the higher excited states (n > 8), and use of different fill and cut-off procedures.¹⁰

References

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T/K	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = P° = 0.1 MPa		log K _f
	C _p ^o	S° - [C _p ^o - F(T _r)/T]	H° - H(T _r)	Δ _f G°	
0	0	INFINITE	-6.197	282.053	INFINITE
100	20.786	151.009	-4.119	269.325	-140.681
200	20.786	165.416	-2.040	283.655	-66.599
250	20.786	170.055	-1.001	283.492	-51.786
298.15	20.786	173.716	0	283.257	-42.223
300	20.786	173.844	0.038	283.247	-41.917
350	20.786	176.949	1.078	282.938	-34.876
400	20.786	179.874	2.117	282.576	-29.600
450	20.786	182.272	3.136	282.147	-25.503
500	20.786	184.462	4.196	281.681	-22.231
600	20.786	188.252	6.274	280.649	-17.335
700	20.786	191.456	8.353	279.461	-13.851
800	20.786	194.232	10.431	278.122	-11.250
900	20.786	196.680	12.510	276.636	-9.237
1000	20.786	198.870	14.589	275.015	-7.639
1100	20.786	200.851	16.657	273.266	-6.347
1200	20.786	202.660	18.746	271.505	-5.279
1300	20.786	204.324	20.824	269.737	-4.379
1400	20.786	205.864	22.903	268.003	-3.616
1500	20.787	207.298	24.982	266.306	-2.968
1600	20.788	208.640	27.061	264.643	-2.428
1700	20.791	209.900	29.139	263.010	-1.961
1800	20.797	211.089	31.219	261.414	-1.550
1900	20.806	212.213	33.299	259.851	-1.186
2000	20.822	213.281	35.380	258.323	-0.862
2100	20.845	214.297	37.464	256.837	-0.572
2200	20.880	215.268	39.550	255.393	-0.312
2300	20.930	216.197	41.640	253.986	-0.076
2334.526	20.951	216.509	42.563	253.548	---
2400	20.987	217.089	43.736	253.076	0
2500	21.083	217.948	45.840	252.568	0
2600	21.198	218.777	47.954	252.023	0
2700	21.341	219.580	50.081	251.441	0
2800	21.515	220.359	52.223	250.823	0
2900	21.726	221.118	54.385	250.170	0
3000	21.976	221.858	56.570	249.583	0
3100	22.269	222.583	58.782	248.957	0
3200	22.606	223.298	61.025	248.293	0
3300	23.000	224.000	63.300	247.590	0
3400	23.424	224.690	65.625	246.848	0
3500	23.909	225.376	67.991	246.068	0
3600	24.445	226.056	70.408	245.248	0
3700	25.034	226.734	72.882	244.388	0
3800	25.675	227.410	75.417	243.488	0
3900	26.370	228.086	78.019	242.548	0
4000	27.118	228.763	80.693	241.568	0
4100	27.919	229.442	83.444	240.548	0
4200	28.772	230.125	86.278	239.488	0
4300	29.678	230.813	89.200	238.388	0
4400	30.635	231.506	92.216	237.248	0
4500	31.574	232.201	95.311	236.068	0
4600	32.606	232.907	98.520	234.848	0
4700	33.681	233.619	101.834	233.588	0
4800	34.798	234.340	105.258	232.298	0
4900	35.956	235.069	108.795	230.978	0
5000	37.153	235.808	112.450	229.628	0
5100	38.389	236.556	116.227	228.248	0
5200	39.664	237.313	120.129	226.838	0
5300	40.976	238.081	124.161	225.398	0
5400	42.327	238.860	128.321	223.928	0
5500	43.716	239.649	132.627	222.428	0
5600	45.144	240.321	136.401	220.898	0
5700	46.624	241.101	140.808	219.338	0
5800	47.714	241.887	145.324	217.748	0
5900	46.784	242.677	149.948	216.128	0
6000	47.832	243.472	154.679	214.478	0

PREVIOUS:

CURRENT: June 1984 (1 bar)

Manganese (Mn)

Mn₁(g)

Manganese, Ion (Mn⁺)

Mn⁺(g)

IP(Mn⁺, g) = 126145.0 ± 0.6 cm⁻¹
 S°(298.15 K) = 174.997 ± 0.05 J K⁻¹ mol⁻¹

ΔH°(0 K) = 999.6 ± 0.5 kJ mol⁻¹
 ΔH°(298.15 K) = [10006.986] kJ mol⁻¹

IDEAL GAS

Electronic Level and Quantum Weights State	ε, cm ⁻¹	g _e
⁷ S ₃	0.00	7
⁵ S ₂	9472.97	5
³ D ₄	14325.86	9
.	.	.
¹ H ₄	120721.9	17
IP	126145.0	

Enthalpy of Formation
 ΔH°(Mn⁺, g, 0 K) is calculated from ΔH°(Mn, g, 0 K) using the spectroscopic value of IP(Mn) = 59981 ± 1 cm⁻¹ (717.532 ± 0.012 mol⁻¹) from Corliss and Sugar.² The ionization limit is converted from cm⁻¹ to kJ mol⁻¹ using the factor, 1 cm⁻¹ = 0.01196266 kJ mol⁻¹, which is derived from the 1973 CODATA fundamental constants,³ Rosenstock *et al.*,⁴ and Levin and Lias⁵ have summarized additional ionization and appearance potential data.
 ΔH°(Mn⁺, g, 298.15 K) is calculated from ΔH°(Mn, g, 0 K) by using IP(Mn) with JANAF¹ enthalpies, H°(0 K) - H°(298.15 K), for Mn(g), Mn⁺(g), and e⁻ (ref). ΔH°(Mn → Mn⁺ + e⁻, 298.15 K) differs from a room temperature threshold energy due to inclusion of these enthalpies and to threshold effects discussed by Rosenstock *et al.*⁴ ΔH°(298.15 K) should be changed by -6.197 kJ mol⁻¹ if it is to be used in the ion convention that excludes the enthalpy of the electron.

Heat Capacity and Entropy

The information on electronic energy levels and quantum weights, given by Corliss and Sugar,² is incomplete because many theoretically predicted levels have not been observed. Although we have listed only the ground, the first excited state, the highest observed excited state, and the ionization potential for Mn⁺(g), all levels listed by Corliss and Sugar,² as well as estimated levels, are used in the calculation. The observed levels are too numerous to list completely. The calculations indicate that for Mn⁺(g), the thermodynamic functions are independent of the estimated missing levels (for n = 4-7), the cut-off procedure, and the inclusion of n < 8 levels up to 6000 K; the Gibbs energy function showing no significant variations at this temperature. The reported uncertainty in S°(298.15 K) is due to uncertainties in the relative ionic mass and the fundamental constants. Extension of these calculations above 6000 K may require consideration of the higher excited states (n > 7), and use of different fill and cut-off procedures.⁶

References

- ¹JANAF Thermochemical Tables: Mn(g), 6-30-84, e⁻ (ref), 3-31-82.
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- ³E. R. Cohen and B. N. Taylor, *J. Phys. Chem. Ref. Data* 2, 663 (1973).
- ⁴H. M. Rosenstock, K. Draxl *et al.*, *J. Phys. Chem. Ref. Data* 6, Supp. 1, 783 pp. (1977).
- ⁵R. D. Levin and S. G. Lias, *U. S. Natl. Bur. Stand., NSRDS-NBS-71*, 634 pp. (1982).
- ⁶J. R. Downey, Jr., *The Dow Chemical Company, AFOSR-TR-78-0960*, Contract No. F44620-75-1-0048, (1978).

T/K	C _p ^o	S ^o - [C _p ^o - F(T)]/RT	H ^o - H ^o (T)	ΔH ^o	log K ₁
	J K ⁻¹ mol ⁻¹	J K ⁻¹ mol ⁻¹	J mol ⁻¹	J mol ⁻¹	
0	0	INFINITE			
100	20.786	152.290	-6.197	999.586	-167.855
200	20.786	166.628	-4.119		-166.767
250	20.786	171.336	-2.040		-161.710
298.15	20.786	174.997	0.	1006.986	-172.904
300	20.786	175.126	0.038		-108.788
400	20.786	178.330	1.078	1007.015	-96.555
500	20.786	181.106	2.117	1008.423	924.219
600	20.786	183.534	3.156	1009.033	889.700
700	20.786	185.744	4.196	1010.653	872.241
800	20.786	187.534	5.234	1011.543	854.699
900	20.786	189.005	6.274	1012.875	837.144
1000	20.787	190.282	7.313	1014.589	819.731
1100	20.790	191.400	8.353	1016.668	802.286
1200	20.795	192.373	9.392	1019.117	784.815
1300	20.805	193.213	10.431	1021.927	767.387
1400	20.821	193.930	11.468	1025.098	750.184
1500	20.846	194.536	12.510	1028.632	733.668
1600	20.882	195.027	13.553	1032.528	717.350
1700	20.932	195.403	14.599	1036.785	701.107
1800	20.996	195.663	15.650	1041.403	684.728
1900	21.078	195.807	16.708	1046.388	668.461
2000	21.179	195.828	17.774	1051.733	652.214
2100	21.301	195.726	18.848	1057.446	635.985
2200	21.445	195.496	19.931	1063.528	619.774
2300	21.611	195.132	21.024	1070.077	603.574
2400	21.800	194.626	22.127	1077.092	587.386
2500	22.011	193.972	23.241	1084.572	571.214
2600	22.246	193.179	24.366	1092.517	555.064
2700	22.507	192.237	25.502	1100.927	538.936
2800	22.796	191.156	26.649	1109.802	522.829
2900	23.080	190.035	27.807	1119.142	506.744
3000	23.398	188.874	28.976	1128.957	490.680
3100	23.751	187.674	30.156	1139.247	474.637
3200	24.138	186.436	31.348	1150.112	458.615
3300	24.559	185.161	32.553	1161.553	442.614
3400	25.014	183.851	33.774	1173.571	426.634
3500	25.523	182.507	35.011	1186.167	410.674
3600	26.070	181.132	36.264	1199.342	394.734
3700	26.657	179.727	37.534	1213.097	378.814
3800	27.284	178.292	38.821	1227.442	362.914
3900	27.951	176.827	40.125	1242.377	347.034
4000	28.660	175.332	41.446	1257.912	331.174
4100	29.411	173.807	42.784	1274.047	315.334
4200	30.204	172.252	44.138	1290.782	299.514
4300	31.041	170.667	45.504	1308.117	283.714
4400	31.924	169.052	46.884	1326.052	267.934
4500	32.853	167.407	48.278	1344.587	252.174
4600	33.828	165.732	49.687	1363.722	236.434
4700	34.849	164.027	51.112	1383.457	220.714
4800	35.916	162.292	52.553	1403.792	205.014
4900	37.029	160.527	54.011	1424.727	189.334
5000	38.288	158.732	55.486	1446.262	173.674
5100	39.693	156.907	56.978	1468.407	158.034
5200	41.254	155.052	58.487	1491.162	142.414
5300	42.971	153.167	59.994	1514.527	126.814
5400	44.844	151.252	61.509	1538.502	111.234
5500	46.874	149.307	63.044	1563.087	95.674
5600	49.069	147.332	64.599	1588.282	80.134
5700	51.429	145.327	66.174	1614.087	64.614
5800	53.954	143.292	67.769	1640.502	49.114
5900	56.644	141.227	69.384	1667.527	33.634
6000	59.499	139.132	71.019	1695.162	18.174

PREVIOUS:

CURRENT: June 1984 (1 bar)