REFERENCE STATE

0	to 2750	K	crystal
2750	to 5130.824	K	liquid
above	5130.824	K	ideal monatomic gas

Refer to the individual tables for details.

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = p° = 0.1 MPa

T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
	J·K⁻¹·mol⁻¹			kJ·mol⁻¹			
0	0.	0.	INFINITE	−5.241	0.	0.	0.
100	17.439	12.558	57.153	−4.460	0.	0.	0.
200	23.091	26.878	38.685	−2.361	0.	0.	0.
250	24.154	32.159	36.867	−1.177	0.	0.	0.
298.15	24.694	36.464	36.464	0.	0.	0.	0.
300	24.711	36.616	36.464	0.046	0.	0.	0.
400	25.393	43.826	37.442	2.553	0.	0.	0.
500	25.899	49.548	39.311	5.118	0.	0.	0.
600	26.347	54.309	41.424	7.731	0.	0.	0.
700	26.769	58.403	43.564	10.387	0.	0.	0.
800	27.183	62.004	45.649	13.084	0.	0.	0.
900	27.593	65.230	47.648	15.823	0.	0.	0.
1000	27.999	68.158	49.555	18.603	0.	0.	0.
1100	28.405	70.846	51.370	21.423	0.	0.	0.
1200	28.798	73.334	53.098	24.284	0.	0.	0.
1300	29.179	75.654	54.745	27.182	0.	0.	0.
1400	29.589	77.831	56.317	30.120	0.	0.	0.
1500	30.062	79.888	57.820	33.102	0.	0.	0.
1600	30.606	81.846	59.261	36.135	0.	0.	0.
1700	31.221	83.719	60.645	39.226	0.	0.	0.
1800	31.903	85.523	61.977	42.381	0.	0.	0.
1900	32.639	87.267	63.263	45.608	0.	0.	0.
2000	33.430	88.961	64.506	48.911	0.	0.	0.
2100	34.275	90.612	65.710	52.296	0.	0.	0.
2200	35.187	92.228	66.878	55.768	0.	0.	0.
2300	36.192	93.813	68.015	59.336	0.	0.	0.
2400	37.317	95.377	69.123	63.010	0.	0.	0.
2500	38.635	96.926	70.204	66.805	0.	0.	0.
2600	40.233	98.471	71.261	70.745	0.	0.	0.
2700	42.283	100.027	72.298	74.868	0.	0.	0.
2750.000	43.423	100.813	72.809	77.011	CRYSTAL <--> LIQUID TRANSITION		
2750.000	33.472	110.596	72.809	103.914			
2800	33.472	111.199	73.489	105.587	0.	0.	0.
2900	33.472	112.374	74.810	108.935	0.	0.	0.
3000	33.472	113.508	76.081	112.282	0.	0.	0.
3100	33.472	114.606	77.306	115.629	0.	0.	0.
3200	33.472	115.669	78.489	118.976	0.	0.	0.
3300	33.472	116.699	79.631	122.323	0.	0.	0.
3400	33.472	117.698	80.736	125.671	0.	0.	0.
3500	33.472	118.668	81.806	129.018	0.	0.	0.
3600	33.472	119.611	82.843	132.365	0.	0.	0.
3700	33.472	120.528	83.849	135.712	0.	0.	0.
3800	33.472	121.421	84.826	139.059	0.	0.	0.
3900	33.472	122.290	85.776	142.407	0.	0.	0.
4000	33.472	123.138	86.699	145.754	0.	0.	0.
4100	33.472	123.964	87.598	149.101	0.	0.	0.
4200	33.472	124.771	88.474	152.448	0.	0.	0.
4300	33.472	125.558	89.327	155.795	0.	0.	0.
4400	33.472	126.328	90.159	159.143	0.	0.	0.
4500	33.472	127.080	90.971	162.490	0.	0.	0.
4600	33.472	127.816	91.764	165.837	0.	0.	0.
4700	33.472	128.536	92.539	169.184	0.	0.	0.
4800	33.472	129.240	93.296	172.531	0.	0.	0.
4900	33.472	129.930	94.037	175.879	0.	0.	0.
5000	33.472	130.607	94.762	179.226	0.	0.	0.
5100	33.472	131.270	95.471	182.573	0.	0.	0.
5130.824	33.472	131.471	95.687	183.605	LIQUID <--> IDEAL GAS FUGACITY = 1 bar		
5130.824	36.434	266.042	95.686	874.064			
5200	36.642	266.531	97.956	876.592	0.	0.	0.
5300	36.943	267.232	101.143	880.271	0.	0.	0.
5400	37.115	267.914	104.225	883.923	0.	0.	0.
5600	37.678	269.274	110.095	891.403	0.	0.	0.
5800	38.251	270.606	115.607	898.995	0.	0.	0.
6000	38.839	271.913	120.795	906.704	0.	0.	0.

PREVIOUS: December 1973 (1 atm) CURRENT: December 1973 (1 bar)

$S°(298.15\ K) = 36.46 \pm 0.4\ J·K^{-1}·mol^{-1}$
$T_{fus} = 2750 \pm 10\ K$

$\Delta_f H°(0\ K) = 0\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = 0\ kJ·mol^{-1}$
$\Delta_{fus} H° = 26.90 \pm 0.8\ kJ·mol^{-1}$

Enthalpy of Formation

Zero by definition.

Heat Capacity and Entropy

The heat capacity values for $T < 10$ are chosen to be the same as those adopted by Hultgren *et al.*[1] A graphical integration of these $C_p°$ data yields $S°(10\ K) = 0.029\ J·K^{-1}·mol^{-1}$ and $H°(10\ K) = 0.19\ cal·mol^{-1}$. The work by DaSilva *et al.*[2,3] on the low temperature (1–10 K) heat capacity of annealed and unannealed niobium wires in magnetic fields supports this choice. Clusius *et al* [4] measured the heat capacity (61 pts.) in the region 11–274 K. This data is smoothed graphically and is constrained to join smoothly with the $C_p°$ values for $T \leq 10$ K. Deviations up to 4% occur between the observed and adopted $C_p°$ values for $T < 80$ K. The deviations here parallel the deviations obtained in our analysis of the heat capacity for Ta.[5] The deviations decrease steadily with increasing temperature up to 274 K.

There are numerous high temperature heat capacity and enthalpy measurements for Nb(cr). The various studies are listed below.

Source	T/K	Method
[6]	273–1873	drop
[7]	454–1882	drop
[8]	433–1840	drop
[9]	1400–2350	modul
[10]	1300–2700	modul
[11]	358–1415	drop
[12]	600–2600	drop
[13]	1273–2593	drop
[14]	1100–2400	pulse
[15]	1500–2700	pulse
[16]	1650–2707	drop

The adopted $C_p°$ values for $T > 298.15$ K are obtained by a combination of graphical and polynomial curve fitting techniques. A polynomial curve fit procedure is used on the enthalpy data of Hawkins and Orr[11] with the constraint that it join smoothly in the 298.15 K region with the enthalpy derived from the Clusius *et al.*[4] heat capacity data. Above 1300 K, a heat capacity curve is adopted through graphical procedures. The adopted curve is chosen so as to be intermediate between the $C_p°$ values of Cezairliyan[15] and the higher $C_p°$ values implied from the enthalpy data of Kirillin *et al.*[12] and Sheindlin *et al.*[16] In general there is good agreement between the various sets of data.

The heat capacity values near T_{fus} are the smoothed values suggested by Cezairliyan.[15] In comparison with the adopted $C_p°$ values, Cezairliyan's smoothed data lies low by 1.9% at 1500 K with the difference steadily decreasing to zero at 2600 K. The smoothed results of Cezairliyan[15] are used for extrapolation to 3200 K. The $C_p°$ values reported by Makarenko and Trukhanov[14] are linear in the region 1100–2400 K whereas the adopted $C_p°$ values are nonlinear; the $C_p°$–T curve being concave upward in this region. The $C_p°$ values of Makarenko *et al.*[14] are within −0.4% to +0.8% of the adopted values in the region 1400– 2100 K but drift to −3% at 1100 K and 2400 K. In comparing enthalpies, Kirillin *et al.*[12] reported smoothed values[2] which are 15 $cal·mol^{-1}$ or 0.8% lower than our tabulated values at 600 K and drift to 849 $cal·mol^{-1}$ or 4.5% higher at 2700 K. The enthalpy results of Sheindlin *et al.*[16] lie above the JANAF values by 0.9% in the region 1700–2700 K (82 $cal·mol^{-1}$ at 1700 K and 181 $cal·mol^{-1}$ at 2700 K).

Fusion Data

Refer to the liquid table for details.

Sublimation Data

$\Delta_{sub} H°(298.15\ K)$ for Nb(cr) = Nb(g) is simply $\Delta_f H°(298.15\ K)$ for Nb(g). Refer to the ideal gas table for details.

References

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[2] J. F. DaSilva, N. W. J. van Duykeren, and Z. Dokoupil. Physica 32, 1253 (1966).
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Continued on page 1693

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

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⁻¹mol⁻¹			kJ·mol⁻¹			
0	0.	0.	INFINITE	−5.241	0.	0.	0.
100	17.439	12.558	57.153	−4.460	0.	0.	0.
200	23.091	26.878	38.685	−2.361	0.	0.	0.
250	24.154	32.159	36.867	−1.177	0.	0.	0.
298.15	24.694	36.464	36.464	0.	0.	0.	0.
300	24.711	36.616	36.464	0.046	0.	0.	0.
350	25.088	40.455	36.766	1.291	0.	0.	0.
400	25.393	43.826	37.442	2.553	0.	0.	0.
450	25.653	46.832	38.322	3.830	0.	0.	0.
500	25.899	49.548	39.311	5.118	0.	0.	0.
600	26.347	54.309	41.424	7.731	0.	0.	0.
700	26.769	58.403	43.564	10.387	0	0.	0.
800	27.183	62.004	45.649	13.084	0.	0.	0.
900	27.593	65.230	47.648	15.823	0.	0.	0.
1000	27.999	68.158	49.555	18.603	0.	0.	0.
1100	28.405	70.846	51.370	21.423	0.	0.	0.
1200	28.798	73.334	53.098	24.284	0.	0.	0.
1300	29.179	75.654	54.745	27.182	0.	0.	0.
1400	29.589	77.831	56.317	30.120	0	0.	0.
1500	30.062	79.888	57.820	33.102	0.	0.	0.
1600	30.606	81.846	59.261	36.135	0.	0.	0.
1700	31.221	83.719	60.645	39.226	0.	0.	0.
1800	31.903	85.523	61.977	42.381	0.	0.	0.
1900	32.639	87.267	63.263	45.608	0.	0.	0.
2000	33.430	88.961	64.506	48.911	0.	0.	0.
2100	34.275	90.612	65.710	52.296	0.	0.	0.
2200	35.187	92.228	66.878	55.768	0	0.	0.
2300	36.192	93.813	68.015	59.336	0.	0.	0.
2400	37.317	95.377	69.123	63.010	0.	0.	0.
2500	38.635	96.926	70.204	66.805	0.	0.	0.
2600	40.233	98.471	71.261	70.745	0	0.	0.
2700	42.283	100.027	72.298	74.868	0.	0.	0.
2750.000	43.423	100.813	72.809	77.011	--- CRYSTAL <--> LIQUID ---		
2800	44.643	101.606	73.316	79.212	−26.375	0.484	−0.009
2900	47.342	103.219	74.319	83.808	−25.126	1.423	−0.026
3000	50.410	104.874	75.310	88.692	−23.589	2.313	−0.040
3100	53.879	106.583	76.291	93.903	−21.725	3.146	−0.053
3200	57.777	108.354	77.265	99.483	−19.494	3.914	−0.064

PREVIOUS: June 1972 CURRENT. December 1973

$S°(298.15\ K)$ = [47.302] $J·K^{-1}·mol^{-1}$
T_{fus} = 2750 ± 10 K

$\Delta_f H°(298.15\ K)$ = [29.647] $kJ·mol^{-1}$
$\Delta_{fus}H°$ = 26.90 ± 0.8 $kJ·mol^{-1}$

Enthalpy of Formation

The enthalpy of formation of Nb(l) at 298.15 K is calculated from that of the crystal by adding $\Delta_{fus}H°$ and the difference in enthalpy, $H°(2750\ K)-H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

The enthalpy measurements on Nb(l) by Sheindlin *et al.*[7] and Margrave[8] do not extend over a sufficiently wide temperature range such that a heat capacity value could be derived. Therefore, the heat capacity for Nb(l) is estimated as 8.0 $cal·K^{-1}·mol^{-1}$ by analogy with other monatomic metals. The entropy at 298.15 K is calculated in a manner analogous to that used in calculating the enthalpy of formation. A glass transition is assumed at 1750 K. The heat capacity values used below 1750 K are those of Nb(cr).

Fusion Data

Melting point determinations for Nb have been numerous, with most reported values in the range 2680–2795 K (IPTS–68 scale). A prime cause for diversity in the results is that the melting point is quite sensitive to impurities, especially gases such as oxygen and nitrogen. These effects have been documented by Schofield[1] and Pemsler.[2] The value chosen is 2750 ± 10 K as reported by Cezairliyan[3] using a subsecond pulse heating method. This value is consistent with the heat capacity values near T_{fus} which are also based on related work by Cezairliyan.[4] Other values in this range (corrected to IPTS–68 scale) are 2746 K by Schofield,[1] 2745 K by Pemsler,[2] and 2738 K by Buehler.[5] Kocherzhinskii and Kobzenko[6] have reported a T_{fus} value of 2793 K, using a sample purified by electron zone fusion.

The value chosen for $\Delta_{fus}H°$ is 6.43 ± 0.20 $kcal·mol^{-1}$ as determined by Cezairliyan[3] using a pulse heating technique. Adopting this value gives consistency between the $C_p°$ values near T_{fus}, $\Delta_{fus}H°$, and T_{fus} as all these values are dependent upon the same heating technique. Sheindlin *et al.*[7] reported $\Delta_{fus}H°$ = 6.597 ± 0.170 $kcal·mol^{-1}$ based on enthalpy measurements on Nb(cr) and Nb(l) obtained from levitation calorimetry techniques. In the vicinity of T_{fus}, the adopted enthalpy vlaues for Nb(cr) and Nb(l) lie roughly 200 $cal·mol^{-1}$ lower than those reported by Sheindlin *et al.*[7] Margrave,[8] also using levitation techniques, reported a value $\Delta_{fus}H°$ = 7.9 $kcal·mol^{-1}$. It is felt that Margrave's value was calculated from a measured enthalpy of Nb(l) at T_{fus} and the enthalpy of Nb(cr) at T_{fus} as suggested by Hultgren *et al.*[9] Our enthalpy vlaues at T_{fus} for Nb(cr) would reduce Margrave's value to roughly 7.4 $kcal·mol^{-1}$ for $\Delta_{fus}H°$.

Martynyuk and Tsapkov[10] measured the enthalpies of Nb(cr) and Nb(l) at the melting point using the method of pulse heating. They reported enthalpy of melting value of 7.98 $kcal·mol^{-1}$ for an Nb sample which was reported to be 99.94% pure. No T_{fus} value was reported.

Vaporization Data

T_{vap} is the temperature at which the Gibbs energy change for the reaction Nb(l) = Nb(g) is zero. The difference between $\Delta_f H°$(Nb, g) and $\Delta_f H°$(Nb, l) at T_{vap} is $\Delta_{vap}H°$. The uncertainty in the boiling point is probably of the order of ± 100 K. Also refer to Nb(g) table.

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[9] R. Hultgren, R. L. Orr, and K. K. Kelley, Supplement to Selected Values of Thermodynamic Properties of Metals and Alloys, Nb table, (January, 1966).
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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

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							
100							
200							
250							
298.15	24.694	47.302	47.302	0.	29.647	26.415	−4.628
300	24.711	47.455	47.302	0.046	29.647	26.395	−4.596
350	25.088	51.293	47.605	1.291	29.647	25.853	−3.858
400	25.393	54.664	48.281	2.553	29.647	25.311	−3.305
450	25.653	57.670	49.160	3.830	29.647	24.770	−2.875
500	25.899	60.386	50.149	5 118	29.647	24.228	−2.531
600	26.347	65.148	52.263	7.731	29.647	23.144	−2.015
700	26.769	69.241	54.403	10.387	29.647	22.060	−1.646
800	27.183	72.842	56.487	13.084	29.647	20.976	−1.370
900	27.593	76.068	58.486	15.823	29.647	19.892	−1.155
1000	27.999	78.996	60.393	18.603	29.647	18.808	−0.982
1100	28.405	81.684	62.208	21.423	29.647	17.725	−0.842
1200	28.798	84.172	63.936	24.284	29.647	16.641	−0.724
1300	29.179	86.492	65.583	27.182	29.647	15.557	−0.625
1400	29.589	88.669	67.155	30.120	29.647	14.473	−0.540
1500	30.062	90.727	68.658	33.102	29.647	13.389	−0.466
1600	30.606	92.684	70.099	36.135	29.647	12.306	−0.402
1700	31.221	94.557	71.483	39.226	29.647	11.222	−0.345
1750.000	31.559	95.467	72.156	40.795	GLASS <--> LIQUID TRANSITION		
1750.000	33.472	95.467	72.156	40.795			
1800	33.472	96.410	72.816	42.469	29.734	10.137	−0.294
1900	33.472	98.220	74.106	45.816	29.854	9.044	−0.249
2000	33.472	99.937	75.355	49.163	29.899	7.948	−0.208
2100	33.472	101.570	76.565	52.510	29.861	6.851	−0.170
2200	33.472	103.127	77.737	55.857	29.736	5.757	−0.137
2300	33.472	104.615	78.874	59.205	29.515	4.672	−0.106
2400	33.472	106.039	79.976	62.552	29.188	3.599	−0.078
2500	33.472	107.406	81.046	65.899	28.740	2.541	−0.053
2600	33.472	108.718	82.085	69.246	28.148	1.504	−0.030
2700	33.472	109.982	83.095	72.593	27.372	0.494	−0.010
2750.000	33.472	110.596	83.590	74.267	--- CRYSTAL <--> LIQUID ---		
2800	33.472	111.199	84.077	75.941	0.	0.	0.
2900	33.472	112.374	85.033	79.288	0.	0.	0.
3000	33.472	113.508	85.963	82.635	0.	0.	0.
3100	33.472	114.606	86.870	85.982	0.	0.	0.
3200	33.472	115.669	87.753	89.329	0.	0.	0.
3300	33.472	116.699	88.615	92.677	0.	0.	0.
3400	33.472	117.698	89.456	96.024	0.	0.	0.
3500	33.472	118.668	90.276	99.371	0.	0.	0.
3600	33.472	119.611	91.078	102.718	0.	0.	0.
3700	33.472	120.528	91.862	106.065	0.	0.	0.
3800	33.472	121.421	92.628	109.413	0.	0.	0.
3900	33.472	122.290	93.377	112.760	0.	0.	0.
4000	33.472	123.138	94.111	116.107	0.	0.	0.
4100	33.472	123.964	94.829	119.454	0.	0.	0.
4200	33.472	124.771	95.532	122.801	0.	0.	0.
4300	33.472	125.558	96.221	126.149	0.	0.	0.
4400	33.472	126.328	96.897	129.496	0.	0.	0.
4500	33.472	127.080	97.559	132.843	0.	0.	0.
4600	33.472	127.816	98.209	136.190	0.	0.	0.
4700	33.472	128.536	98.847	139.537	0.	0.	0.
4800	33.472	129.240	99.473	142.885	0.	0.	0.
4900	33.472	129.931	100.087	146.232	0.	0.	0.
5000	33.472	130.607	100.691	149.579	0.	0.	0.
5100	33.472	131.270	101.284	152.926	0.	0.	0.
5130.824	33.472	131.471	101.465	153.958	----- FUGACITY = 1 bar -----		
5200	33.472	131.920	101.867	156.273	−690.672	9.309	−0.094
5300	33.472	132.557	102.440	159.621	−691.004	22.774	−0.224
5400	33.472	133.183	103.004	162.968	−691.309	36.240	−0.351
5600	33.472	134.400	104.103	169.662	−692.094	63.200	−0.590
5800	33.472	135.575	105.168	176.357	−692.992	90.191	−0.812
6000	33.472	136.709	106.201	183.051	−694.007	117.214	−1.020

PREVIOUS: June 1972 CURRENT: December 1973

CRYSTAL-LIQUID

0 to 2750 K crystal
above 2750 K liquid

Refer to the individual tables for details.

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = p° = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
0	0.	0.	INFINITE	−5.241	0	0.	0.
100	17.439	12.558	57.153	−4.460	0.	0.	0.
200	23.091	26.878	38.685	−2.361	0.	0.	0.
250	24.154	32.159	36.867	−1.177	0.	0.	0.
298.15	24.694	36.464	36.464	0.	0.	0.	0.
300	24.711	36.616	36.464	0.046	0.	0.	0.
350	25.088	40.455	36.766	1.291	0.	0.	0.
400	25.393	43.826	37.442	2.553	0.	0.	0.
450	25.653	46.832	38.322	3.830	0.	0.	0.
500	25.899	49.548	39.311	5.118	0.	0.	0.
600	26.347	54.309	41.424	7.731	0.	0.	0.
700	26.769	58.403	43.564	10.387	0.	0.	0.
800	27.183	62.004	45.649	13.084	0.	0.	0.
900	27.593	65.230	47.648	15.823	0.	0.	0.
1000	27.999	68.158	49.555	18.603	0.	0.	0.
1100	28.405	70.846	51.370	21.423	0.	0.	0.
1200	28.798	73.334	53.098	24.284	0.	0.	0.
1300	29.179	75.654	54.745	27.182	0.	0.	0.
1400	29.589	77.831	56.317	30.120	0.	0.	0.
1500	30.062	79.888	57.820	33.102	0.	0.	0.
1600	30.606	81.846	59.261	36.135	0.	0.	0.
1700	31.221	83.719	60.645	39.226	0.	0.	0.
1800	31.903	85.523	61.977	42.381	0.	0.	0.
1900	32.639	87.267	63.263	45.608	0.	0.	0.
2000	33.430	88.961	64.506	48.911	0.	0.	0.
2100	34.275	90.612	65.710	52.296	0.	0.	0.
2200	35.187	92.228	66.878	55.768	0.	0.	0.
2300	36.192	93.813	68.015	59.336	0.	0.	0.
2400	37.317	95.377	69.123	63.010	0.	0.	0.
2500	38.635	96.926	70.204	66.805	0.	0.	0.
2600	40.233	98.471	71.261	70.745	0.	0.	0.
2700	42.283	100.027	72.298	74.868	0.	0.	0.
2750.000	43.423	100.813	72.809	77.011	CRYSTAL <--> LIQUID TRANSITION		
2750.000	33.472	110.596	72.809	103.914			
2800	33.472	111.199	73.489	105.587	0.	0.	0.
2900	33.472	112.374	74.810	108.935	0.	0.	0.
3000	33.472	113.508	76.081	112.282	0.	0.	0.
3100	33.472	114.606	77.306	115.629	0.	0.	0.
3200	33.472	115.669	78.489	118.976	0.	0.	0.
3300	33.472	116.699	79.631	122.323	0.	0.	0.
3400	33.472	117.698	80.736	125.671	0.	0.	0.
3500	33.472	118.668	81.806	129.018	0.	0.	0.
3600	33.472	119.611	82.843	132.365	0.	0.	0.
3700	33.472	120.528	83.849	135.712	0.	0.	0.
3800	33.472	121.421	84.826	139.059	0.	0.	0.
3900	33.472	122.290	85.776	142.407	0.	0.	0.
4000	33.472	123.138	86.699	145.754	0.	0.	0.
4100	33.472	123.964	87.598	149.101	0.	0.	0.
4200	33.472	124.771	88.474	152.448	0.	0.	0.
4300	33.472	125.558	89.327	155.795	0.	0.	0.
4400	33.472	126.328	90.159	159.143	0.	0.	0.
4500	33.472	127.080	90.971	162.490	0.	0.	0.
4600	33.472	127.816	91.764	165.837	0.	0.	0.
4700	33.472	128.536	92.539	169.184	0.	0.	0.
4800	33.472	129.240	93.296	172.531	0.	0.	0.
4900	33.472	129.930	94.037	175.879	0.	0.	0.
5000	33.472	130.607	94.762	179.226	0.	0.	0.
5100	33.472	131.270	95.471	182.573	0.	0.	0.
5130.824	33.472	131.471	95.687	183.605	FUGACITY = 1 bar		
5200	33.472	131.920	96.166	185.920	−690.672	9.310	−0.094
5300	33.472	132.557	96.846	189.267	−691.004	22.774	−0.224
5400	33.472	133.183	97.513	192.615	−691.309	36.240	−0.351
5600	33.472	134.400	98.809	199.309	−692.094	63.200	−0.590
5800	33.472	135.575	100.057	206.003	−692.992	90.191	−0.812
6000	33.472	136.709	101.260	212.698	−694.007	117.214	−1.020

PREVIOUS: CURRENT December 1973

IP(Nb, g) = 55511 ± 1 cm^{-1}
$S°(298.15\ K)$ = 186.26 ± 0.4 $J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K)$ = 729.9 ± 8 $kJ·mol^{-1}$
$\Delta_f H°(298.15\ K)$ = 733.0 ± 8 $kJ·mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^6D_{1/2}$	0.00	2
$^6D_{3/2}$	154.19	4
$^6D_{5/2}$	391.99	6
$^6D_{7/2}$	695.25	8
$^6D_{9/2}$	1050.26	10

Enthalpy of Formation

A 2nd and 3rd law analysis of six reported vapor pressure studies is tabulated below. Five studies[1-5] used the Langmuir free evaporation method while one study[6] used the integral variation of the Knudsen method.

Source	Reaction	T/K (IPTS–68)	Data Points	$\Delta_f H°$(298.15 K), kcal·mol^{-1} 2nd law	3rd law	Drift cal·K^{-1}·mol^{-1}	$\Delta_f H°$ (298.15 K) kcal·mol^{-1}
1	A	2744–3146	15*	146.2	168 4	7.5 ± 1.5	175.5
2	B	2307–2600	14**	175.8	172.5	−1.3 ± 1.6	172.5
3	B	2456–2691	8	182.8	175.7	−2.8 ± 5.3	175.7
4	B	2253–260	eqn	183.4	174.8	−3.6	174.8
5	B	2370–2685	eqn	175.0	177.7	1.1	177.7
6	B	2553–2684	4	143.1	191.4	18.4 ± 4.8	191.4

* 2939.9 K point deleted due to a statistical test.
** 2307, 2328, 2584 K points deleted due to a statistical test.
A = vaporization
B = sublimation

We adopt $\Delta_f H°(298.15\ K)$ = 175.2 kcal·mol^{-1} for Nb(g) which is a rounded average of four results.[2-5] With a drift of 7.5 cal·K^{-1}·mol^{-1} in that data, Shchukarev *et al.*[7] reported an enthalpy of sublimation of Nb(cr), determined at 2243–2393 K,of 172 ± 5 kcal·mol^{-1}. Our tabulations give $\Delta_{sub} H°(2300\ K)$ = 173.5 kcal·mol^{-1}. The same workers[7] later reported $\Delta_{sub} H°(298.15K)$ = 173 kcal·mol^{-1} based on a 2nd law analysis of Nb^+ ion currents at temperatures above 2573 K.

Heat Capacity and Entropy

The electronic levels and quantum weights are obtained from Moore.[8] Only a few of the levels are listed above. All levels reported by Moore[8] are considered in the calculation. There are predicted electronic levels which have not beenobserved.[8] These levels are assumed to lie above 20,000 cm^{-1} and thus will not significantly affect the entropy attemperatures below 3000 K. The heat capacity and entropy values are very similar to those adopted by Hultgren *et al.*,[9] being the sameat 298.15 K and differing by 0.39 cal·K^{-1}·mol^{-1} in C_p at 5500 K.

References

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Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ (J·K^{-1}·mol^{-1})	$S°$ (J·K^{-1}·mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}·mol^{-1})	$H°-H°(T_r)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	$\Delta_f G°$ (kJ·mol^{-1})	log K_f
0	0.	0.	INFINITE	−8.354	729.923	729.923	INFINITE
100	28.819	153.823	212.891	−5.907	731.590	717.463	−374.764
200	29.932	174.240	189.016	−2.955	732.443	702.971	−183.597
250	30.144	180.945	186.756	−1.453	732.761	695.565	−145.330
298.15	30.159	186.259	186.259	0.	733.037	688.375	−120.600
300	30.155	186.446	186.260	0.056	733.047	688.098	−119.809
350	29.969	191.082	186.626	1.560	733.305	680.586	−101.572
400	29.646	195.064	187.438	3.050	733.534	673.039	−87.890
450	29.253	198.534	188.482	4.523	733.730	665.464	−77.245
500	28.840	201.594	189.644	5.975	733.894	657.870	−68.727
600	28.050	206.781	192.083	8.819	734.125	642.642	−55.947
700	27.365	211.052	194.497	11.589	734.239	627.384	−46.816
800	26.785	214.668	196.798	14.296	734.248	612.117	−39.967
900	26.294	217.793	198.961	16.949	734.162	596.855	−34.641
1000	25.880	220.542	200.984	19.557	733.991	581.607	−30.380
1100	25.533	222.991	202.876	22.127	733.741	566.380	−26.895
1200	25.248	225.200	204.646	24.666	733.419	551.179	−23.992
1300	25.023	227.212	206.305	27.179	733.033	536.008	−21.537
1400	24.857	229.060	207.866	29.672	732.589	520.869	−19.434
1500	24.748	230.771	209.336	32.152	732.087	505.763	−17.612
1600	24.696	232.366	210.726	34.624	731.526	490.693	−16.019
1700	24.700	233.863	212.044	37.093	730.904	475.659	−14.615
1800	24.759	235.276	213.296	39.566	730.221	460.664	−13.368
1900	24.872	236.618	214.488	42.047	729.475	445.709	−12.253
2000	25.034	237.898	215.627	44.542	728.667	430.794	−11.251
2100	25.244	239.124	216.717	47.055	727.796	415.922	−10.345
2200	25.496	240.304	217.762	49.592	726.860	401.092	−9.523
2300	25.788	241.444	218.767	52.156	725.856	386.307	−8.773
2400	26.115	242.548	219.735	54.751	724.777	371.567	−8.087
2500	26.472	243.621	220.669	57.380	723.611	356.873	−7.456
2600	26.854	244.667	221.572	60.046	722.338	342.229	−6.875
2700	27.256	245.688	222.446	62.751	720.920	327.635	−6.338
2800	27.675	246.686	223.294	65.498	692.947	313.582	−5.850
2900	28.105	247.665	224.118	68.287	692.389	300.044	−5.404
3000	28.544	248.625	224.919	71.119	691.874	286.523	−4.989
3100	28.986	249.568	225.699	73.995	691.403	273.020	−4.600
3200	29.430	250.496	226.459	76.916	690.977	259.530	−4.236
3300	29.871	251.408	227.202	79.881	690.595	246.054	−3.895
3400	30.309	252.306	227.927	82.890	690.257	232.588	−3.573
3500	30.740	253.191	228.636	85.943	689.962	219.131	−3.270
3600	31.162	254.063	229.330	89.038	689.710	205.683	−2.984
3700	31.576	254.922	230.010	92.175	689.500	192.241	−2.714
3800	31.979	255.770	230.677	95.353	689.330	178.804	−2.458
3900	32.371	256.606	231.331	98.570	689.201	165.370	−2.215
4000	32.751	257.430	231.973	101.827	689.110	151.940	−1.984
4100	33.120	258.243	232.604	105.120	689.056	138.512	−1.765
4200	33.479	259.046	233.224	108.450	689.039	125.084	−1.556
4300	33.826	259.838	233.834	111.816	689.057	111.656	−1.356
4400	34.164	260.619	234.434	115.215	689.110	98.228	−1.166
4500	34.493	261.391	235.024	118.648	689.195	84.798	−0.984
4600	34.814	262.152	235.606	122.114	689.313	71.365	−0.810
4700	35.127	262.904	236.179	125.611	689.463	57.930	−0.644
4800	35.436	263.647	236.743	129.139	689.644	44.492	−0.484
4900	35.740	264.381	237.300	132.698	689.856	31.049	−0.331
5000	36.041	265.106	237.849	136.287	690.098	17.601	−0.184
5100	36.342	265.823	238.390	139.906	690.370	4 149	−0.042
5130.824	36.434	266.042	238.556	141.028	----- FUGACITY = 1 bar -----		
5200	36.642	266.531	238.925	143.555	0.	0.	0.
5300	36.943	267.232	239.452	147.234	0.	0.	0.
5400	37.115	267.914	239.972	150.887	0.	0.	0.
5500	37.396	268.598	240.486	154.612	0.	0.	0.
5600	37.678	269.274	240.994	158.366	0.	0.	0.
5700	37.963	269.943	241.496	162.148	0.	0.	0.
5800	38.251	270.606	241.993	165.959	0.	0.	0.
5900	38.543	271.263	242.483	169.798	0.	0.	0.
6000	38.839	271.913	242.968	173.667	0.	0.	0.

PREVIOUS: December 1973 (1 atm) — CURRENT: December 1973 (1 bar)

IP(Nb^+, g) = 115500 ± 100 cm^{-1}
$S°$(298.15 K) = 183.333 ± 0.4 $J·K^{-1}·mol^{-1}$

$\Delta_f H°$(0 K) = 1394.0 ± 8 $kJ\ mol^{-1}$
$\Delta_f H°$(298.15 K) = [1402.954] $kJ·mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^5D_0$	0.00	1
$^5D_1$	158.38	3
$^5D_2$	438.99	5
$^5D_3$	801.38	7
$^5D_4$	1224.87	9

Enthalpy of Formation

$\Delta_f H°(Nb^+, g, 0\ K)$ is calculated from $\Delta_f H°(Nb, g, 0\ K)$[1] using the spectroscopic value of IP(Nb) = 55511 ± 1 cm^{-1} (664.059 ± 0.01 $kJ·mol^{-1}$) from Moore.[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 Lias[5] have summarized additional ionization and appearance potential data.

$\Delta_f H°(Nb^+, g, 298.15\ K)$ is calculated from $\Delta_f H°(Nb, g, 0\ K)$ by using IP(Nb) with JANAF[1] enthalpies, $H°(0\ K)-H°(298.15\ K)$, for Nb(g), $Nb^+(g)$, and e^-(ref). $\Delta_f H°(Nb \rightarrow Nb^+ + e^-, 298.15\ K)$ differs from a room temperature threshold energy due to inclusion of these enthalpies and to threshold effects discussed by Rosenstock *et al.*[4] $\Delta_f H°(298.15\ K)$ 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 Moore,[6] 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 $Nb^+(g)$, all levels listed by Moore[6] as well as estimated levels, are used in the calculation. The observed levels are too numerous to list completely. The calculations indicate that for $Nb^+(g)$, the thermodynamic functions are independent of the estimated missing levels (for n = 4, 5), the cut-off procedure, and the inclusion of n = 5 levels up to 6000 K; the Gibbs energy function showing variations of 0.2% 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 > 5), and use of different fill and cut-off procedures.[7]

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J·K^{-1}·mol^{-1}$			$kJ·mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−8.015	1393.983		
100	26.964	152.351	209.002	−5.665			
200	28.783	171.684	186.012	−2.866			
250	29.250	178.162	183.816	−1.414			
298.15	29.421	183.333	183.333	0.	1402.954	1352.911	−237.024
300	29.423	183.515	183.333	0.054	1403.002	1352.600	−235.509
350	29.331	188.046	183.691	1.524	1404.265	1344.099	−200.596
400	29.059	191.947	184.485	2.985	1405.503	1335.419	−174.388
450	28.698	195.349	185.507	4.429	1406.710	1326.586	−153.986
500	28.323	198.353	186.645	5.854	1407.886	1317.620	−137.651
600	27.697	203.458	189.036	8.653	1410.151	1299.353	−113.119
700	27.316	207.696	191.407	11.402	1412.322	1280.714	−95.568
800	27.143	211.330	193.676	14.123	1414.425	1261.768	−82.385
900	27.099	214.524	195.819	16.835	1416.476	1242.562	−72.116
1000	27.118	217.380	197.834	19.545	1418.485	1223.131	−63.890
1100	27.159	219.966	199.731	22.259	1420.457	1203.499	−57.149
1200	27.203	222.331	201.517	24.977	1422.394	1183.690	−51.525
1300	27.242	224.510	203.203	27.700	1424.296	1163.721	−46.759
1400	27.281	226.530	204.798	30.426	1426.163	1143.606	−42.668
1500	27.324	228.414	206.310	33.156	1427.990	1123.360	−39.119
1600	27.378	230.179	207.747	35.891	1429.771	1102.993	−36.009
1700	27.448	231.841	209.116	38.632	1431.500	1082.516	−33.262
1800	27.537	233.412	210.423	41.381	1433.171	1061.939	−30.817
1900	27.647	234.904	211.672	44.140	1434.782	1041.271	−28.627
2000	27.780	236.325	212.870	46.911	1436.329	1020.519	−26.653
2100	27.934	237.684	214.019	49.697	1437.809	999.692	−24.866
2200	28.108	238.988	215.125	52.499	1439.217	978.796	−23.240
2300	28.300	240.242	216.190	55.319	1440.548	957.838	−21.753
2400	28.507	241.450	217.217	58.159	1441.793	936.823	−20.389
2500	28.726	242.618	218.210	61.021	1442.938	915.759	−19.134
2600	28.956	243.750	219.171	63.905	1443.961	894.651	−17.974
2700	29.193	244.847	220.101	66.812	1444.823	873.507	−16.899
2800	29.437	245.913	221.004	69.744	1419.114	852.819	−15.910
2900	29.686	246.950	221.881	72.700	1420.802	832.564	−14.996
3000	29.939	247.961	222.734	75.681	1422.514	812.251	−14.143
3100	30.196	248.947	223.563	78.688	1424.252	791.880	−13.343
3200	30.457	249.909	224.372	81.720	1426.016	771.453	−12.593
3300	30.723	250.851	225.160	84.779	1427.807	750.970	−11.887
3400	30.996	251.772	225.929	87.865	1429.624	730.433	−11.222
3500	31.276	252.674	226.680	90.979	1431.469	709.842	−10.594
3600	31.566	253.560	227.415	94.121	1433.343	689.197	−10.000
3700	31.868	254.429	228.133	97.292	1435.246	668.500	−9.438
3800	32.183	255.283	228.837	100.495	1437.179	647.752	−8.904
3900	32.513	256.123	229.525	103.729	1439.145	626.952	−8.397
4000	32.861	256.950	230.201	106.998	1441.145	606.101	−7.915
4100	33.229	257.766	230.863	110.302	1443.181	585.200	−7.456
4200	33.617	258.571	231.513	113.644	1445.255	564.248	−7.017
4300	34.027	259.367	232.152	117.027	1447.368	543.247	−6.599
4400	34.461	260.154	232.779	120.451	1449.524	522.196	−6.199
4500	34.917	260.934	233.396	123.919	1451.724	501.096	−5.817
4600	35.398	261.707	234.003	127.435	1453.971	479.946	−5.450
4700	35.902	262.473	234.601	131.000	1456.267	458.747	−5.098
4800	36.428	263.235	235.190	134.616	1458.615	437.498	−4.761
4900	36.977	263.991	235.770	138.286	1461.016	416.200	−4.437
5000	37.546	264.744	236.342	142.012	1463.473	394.853	−4.125
5100	38.133	265.493	236.906	145.796	1465.989	373.456	−3.825
5200	38.737	266.240	237.463	149.639	777.892	361.318	−3.629
5300	39.356	266.983	238.013	153.544	780.196	353.285	−3.482
5400	39.985	267.725	238.556	157.511	782.589	345.204	−3.339
5500	40.624	268.464	239.093	161.541	784.972	337.082	−3.201
5600	41.268	269.202	239.624	165.636	787.392	328.917	−3.068
5700	41.915	269.938	240.150	169.795	789.847	320.708	−2.939
5800	42.561	270.673	240.670	174.019	792.339	312.456	−2.814
5900	43.203	271.406	241.184	178.307	794.866	304.160	−2.693
6000	43.839	272.137	241.694	182.659	797.428	295.822	−2.575

PREVIOUS: CURRENT. March 1984 (1 bar)

EA(Nb, g) = 0.893 ± 0.025 eV
$S°(298.15\ K)$ = 186.095 ± 0.002 $J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K)$ = 643.763 ± 4.5 $kJ·mol^{-1}$
$\Delta_f H°(298.15\ K)$ = [640.978] $kJ·mol^{-1}$

Electonic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^5D_0$	0	1
$^5D_1$	110	3
$^5D_2$	310	5
$^5D_3$	560	7
$^5D_4$	870	9

Enthalpy of Formation

$\Delta_f H°(Nb^-, g, 0\ K)$ is calculated from $\Delta_f H°(Nb, g, 0\ K)$[1] using the adopted electron affinity of EA(Nb) = 0.893 ± 0.025 eV (86.161 ± 2.412 $kJ·mol^{-1}$). This value, recommended by Hotop and Lineberger,[2] is based on a laser photodetachment electron spectrometry study.[3] Additional information on Nb^-(g) may be obtained in the critical discussions of Hotop and Lineberger,[2, 4] Rosenstock *et al.*[5] and Massey.[6]

$\Delta_f H°(Nb^-, g, 298.15\ K)$ is obtained from $\Delta_f H°(Nb, g, 0\ K)$ by using EA(Nb) with JANAF[1] enthalpies, $H°(0\ K)-H°(298.15\ K)$, or Nb^-(g), Nb(g), and e^-(ref). $\Delta_r H°(Nb^- \rightarrow Nb + e^-, 298.15\ K)$ differs from a room-temperature threshold energy due to inclusion of these enthalpies and to threshold effects discussed by Rosenstock *et al.*[5] $\Delta_f H°(298.15\ K)$ 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 ground state electronic configuration for Nb^-(g) is given by Hotop and Lineberger,[2, 4] Rosenstock *et al.*,[5] and Massey.[6] The fine structure separation has been calculated by an isoelectronic extrapolation of ratios of fine structure separations[3] and is that recommended by Hotop and Lineberger.[2]

References

[1]JANAF Thermochemical Tables: Nb(g), 12–31–73, e^-(ref), 3–31–82.
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[5]H. M. Rosenstock, K. Draxl *et al.* J. Phys. Chem. Ref. Data 6, Supp. 1, 783 pp. (1977).
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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J·K^{-1}·mol^{-1}$			$kJ·mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−8.654	643.763		
100	30.251	153.166	212.710	−5.954			
200	30.317	174.205	188.796	−2.918			
250	29.768	180.919	186.576	−1.414			
298.15	28.948	186.095	186.095	0.	640.978	602.621	−105.577
300	28.913	186.274	186.095	0.054	640.948	602.383	−104.884
350	27.956	190.659	186.444	1.475	640.085	596.023	−88.952
400	27.029	194.331	187.207	2.850	639.158	589.790	−77.019
450	26.196	197.465	188.177	4.180	638.172	583.678	−67.752
500	25.474	200.187	189.245	5.471	637.135	577.678	−60.350
600	24.342	204.725	191.461	7.959	634.932	565.991	−49.274
700	23.538	208.414	193.627	10.350	632.589	554.685	−41.391
800	22.962	211.517	195.675	12.674	630.136	543.722	−35.501
900	22.541	214.196	197.587	14.948	627.593	533.072	−30.939
1000	22.227	216.554	199.368	17.186	624.972	522.709	−27.304
1100	21 988	218.661	201.028	19.396	622.284	512.613	−24.342
1200	21.803	220.566	202.578	21.585	619.534	502.764	−21.885
1300	21.656	222.305	204.030	23.758	616.729	493.146	−19.815
1400	21.539	223.905	205.393	25.917	613.872	483.746	−18.049
1500	21.443	225.388	206.677	28.066	610.961	474.553	−16.525
1600	21.364	226.769	207.890	30.206	607.990	465.556	−15.199
1700	21.299	228.062	209.039	32.339	604.953	456.746	−14.034
1800	21.243	229.278	210.130	34.466	601.846	448.117	−13.004
1900	21.197	230.425	211.168	36.588	598.663	439.663	−12.087
2000	21.157	231.512	212.159	38.706	595.399	431.379	−11.266
2100	21.122	232.543	213.105	40.820	592.049	423.260	−10.528
2200	21.092	233.525	214.011	42.931	588.609	415.303	−9.861
2300	21.066	234.462	214.880	45.038	585.070	407.504	−9.255
2400	21.043	235.358	215.715	47.144	581.423	399.862	−8.703
2500	21.023	236.217	216.518	49.247	577.653	392.374	−8.198
2600	21.005	237.041	217.291	51.349	573.736	385.039	−7.736
2700	20.989	237.833	218.038	53.448	569.634	377.859	−7.310
2800	20.975	238.596	218.758	55.546	538.934	371.319	−6.927
2900	20.962	239.332	219.455	57.643	535.605	365.391	−6.581
3000	20.950	240.043	220.130	59.739	532.275	359.579	−6.261
3100	20.940	240.729	220.783	61.833	528.944	353.877	−5.963
3200	20.930	241.394	221.417	63.927	525.611	348.283	−5.685
3300	20.922	242.038	222.032	66.019	522.278	342.793	−5.426
3400	20.914	242.662	222.630	68.111	518.944	337.404	−5.184
3500	20.906	243.268	223.211	70.202	515.609	332.113	−4.957
3600	20.900	243.857	223.776	72.293	512.274	326.918	−4 743
3700	20.894	244.430	224.327	74.382	508.938	321.815	−4.543
3800	20.888	244.987	224.863	76.471	505.601	316.802	−4.355
3900	20.883	245.530	225.386	78.560	502.264	311.877	−4.177
4000	20.878	246.058	225.896	80.648	498.926	307.038	−4.010
4100	20.874	246.574	226.394	82.735	495.588	302.282	−3.851
4200	20.869	247.077	226.881	84.823	492.249	297.608	−3.701
4300	20.866	247.568	227.356	86.909	488.910	293.013	−3.559
4400	20.862	248.047	227.821	88.996	485.570	288.496	−3.425
4500	20.859	248.516	228.276	91.082	482.231	284.054	−3.297
4600	20.855	248.974	228.721	93.167	478.891	279.687	−3.176
4700	20.853	249.423	229.156	95.253	475.550	275.393	−3.061
4800	20.850	249.862	229.583	97.338	472.210	271.169	−2.951
4900	20.847	250.292	230.001	99.423	468.869	267.016	−2.846
5000	20.845	250.713	230.412	101.507	465.527	262.930	−2.747
5100	20.842	251.126	230.814	103.592	462.186	258.911	−2.652
5200	20.840	251.530	231.208	105.676	−231.828	264.268	−2.655
5300	20.838	251.927	231.595	107.760	−235.501	273.843	−2.699
5400	20.836	252.317	231.975	109.844	−239.149	283.483	−2.742
5500	20.834	252.699	232.349	111.927	−242.869	293.196	−2.785
5600	20.833	253.075	232.716	114.010	−246.618	302.977	−2.826
5700	20.831	253 443	233.076	116.094	−250.396	312.824	−2.867
5800	20.830	253.806	233.430	118.177	−254.202	322.738	−2.907
5900	20.828	254.162	233.779	120.260	−258.037	332.718	−2.946
6000	20.827	254.512	234.121	122.342	−261.902	342.764	−2.984

PREVIOUS: CURRENT: March 1984 (1 bar)

$S°(298.15\ K) = [46.024 \pm 8.4]\ J·K^{-1}·mol^{-1}$
$T_{fus} = 2210 \pm 15\ K$

$\Delta_f H°(0\ K)$ = Unknown
$\Delta_f H°(298.15\ K) = -419.66 \pm 12.6\ kJ·mol^{-1}$
$\Delta_{fus} H° = 85.354 \pm 20.9\ kJ·mol^{-1}$
$\Delta_{sub} H°(298.15\ K) = 618.395 \pm 20.9\ kJ·mol^{-1}$

Enthalpy of Formation

There are two reported oxygen bomb calorimetric studies for NbO(cr). The results must be interpreted in light of impure samples, incomplete combustion to Nb_2O_5(cr), and the possible nonstoichiometry of the reactants and products. Morozova and Getskina[1] reported $\Delta_c H°(291\ K) = 255.0\ kcal·mol^{-1}$ while Kusenko and Gel'd[2] reported $\Delta_c H°(298.15\ K) = 263.2\ kcal·mol^{-1}$ for the combustion of NbO(cr). Using auxiliary data,[3] we calculate $\Delta_f H°(298.15\ K) = -99.5$ and $-95.4\ kcal·mol^{-1}$ for NbO(cr).Schaefer and Liedmeier,[4] using Cl_2 bomb calorimetry, reported a value of $-97 \pm 1\ kcal·mol^{-1}$, based on $\Delta_f H°(NbOCl_3, cr, 298.15\ K) = -210.2\ kcal·mol^{-1}$.

A 2nd and 3rd law analysis of the majority of the reported smoothed emf data is tabulated below. Note that the enthalpy of formation for NbO(cr) calculated from the 3rd law $\Delta_r H°$ values are roughly 3 $kcal·mol^{-1}$ more negative than the adopted value. There is, however, excellent agreement within the equilibrium data; the 3rd law $\Delta_f H°(298.15\ K)$ values average $-100.3\ kcal·mol^{-1}$ with a spread of only 1.8 $kcal·mol^{-1}$. We adopt $\Delta_f H°(298.15\ K) = 100.3 \pm 3.0\ kcal·mol^{-1}$ based on an average of the equilibrium studies.[5-11] The reason for the discrepancy between the equilbrium and combustion results is not known at this time.[8]

Source	T/K	Reaction	$\Delta_f H°(298.15\ K)$, $kcal·mol^{-1}$ 2nd law	3rd law	Drift $cal·K^{-1}·mol^{-1}$	$\Delta_f H°(298.15\ K)$ $kcal·mol^{-1}$
[5]	1245–1379	A	−35.56	−36.38	−0.63	−100.02
[6]	1115–1347	A	−35.34	−37.60	−1.80	−101.24
[7]	1123–1323	A	−38.62	−36.20	1.98	−99.84
[8]	1030–1300	B	−11.17	3.19	6.62	−100.99
[9]	1000–1400	A	−37.82	−35.91	1.60	−99.55
[10]	1073–1373	A	−36.95	−36.46	0.40	−100.10
[11]	1177–1388	C	−9.69	−9.72	−0.03	−100.12

A) $Nb(cr) + Fe_{0.95}O = NbO(cr) + 0.95\ Fe(cr)$
B) $Nb(cr) + 0.2\ Ta_2O_5(cr) = 0.4\ Ta(cr) + NbO(cr)$
C) $Nb(cr) + 1/3\ Cr_2O_3(cr) = NbO(cr) + 2/3\ Cr(cr)$

Heat Capacity and Entropy

Gel'd and Kusenko[12] measured the enthalpy of NbO(cr) and reported fourteen data points in the range 420–1702 K (IPTS–68). A Shomate type equation is used to represent the data. The average deviation between the data and calculated values is 0.31%; the maximum deviation of 0.62% occurs at 1518 K. This equation is used to obtain extrapolated values of $C_p°$ up to T_{fus}.

There is no low temperature heat capacity data reported in the literature for $T < 298$ K. In order to have the 3rd law results of the equilibrium data agree with the combustion data, an entropy value of the order of 13–14 $cal·K^{-1}·mol^{-1}$ would be necessary. At this point, however, the 3rd law drifts would be all positive. $S°(298.15\ K) = 10.2\ cal·K^{-1}·mol^{-1}$ would lead to a more satisfying variation in the 3rd law drifts for the condensed phase equilibrium data but an intermediate value $S°(298.15\ K) = 11.0\ cal·K^{-1}·mol^{-1}$ gives better consistency with the vapor pressure data. For more details refer to the NbO(g) and NbO_2(g) tables.[3]

Phase Data

Brauer[13] reported a homogeneity range of $x = 0.89–1.04$ for NbO_x. NbO(cr) has a cubic structure, a NaCl type with ordered vacancies.[13,14] Further information may be found in the review of the Nb–O system by Elliott.[15]

Fusion Data

Refer to the liquid table for details.

Sublimation Data

The mass spectrometric study by Shchukarev *et al.*[16] indicated that NbO(cr) at elevated temperatures yields NbO(g) and NbO_2(g). In the range 1873–2473 K, the concentration of NbO in the vapor phase over NbO(cr, l) varied in the range 5–30%.[16] $\Delta_{sub} H°(298.15\ K) = 147.8 \pm 5.0\ kcal·mol^{-1}$ is calculated as the difference between the $\Delta_f H°(298.15\ K)$ values for NbO(g) and NbO(cr).

References

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Continued on page 1693

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

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						
100						
200						
250						
298.15	41.112	46.024	46.024	0.	−419.655	−391.923	68.663
300	41.187	46.279	46.025	0.076	−419.652	−391.751	68.210
400	44.032	58.555	47.679	4.350	−419.371	−382.488	49.948
500	45.827	68.584	50.888	8.848	−418.968	−373.313	39.000
600	47.204	77.064	54.562	13.501	−418.507	−364.224	31.709
700	48.369	84.429	58.314	18.280	−418.011	−355.216	26.507
800	49.467	90.960	61.994	23.173	−417.485	−346.281	22.610
900	50.481	96.845	65.545	28.170	−416.929	−337.414	19.583
1000	51.467	102.215	68.947	33.268	−416.342	−328.610	17.165
1100	52.418	107.165	72.199	38.462	−415.722	−319.866	15.189
1200	53.359	111.766	75.307	43.751	−415.068	−311.181	13.545
1300	54.287	116.074	78.279	49.134	−414.376	−302.551	12.157
1400	55.208	120.131	81.125	54.608	−413.646	−293.976	10.968
1500	56.117	123.971	83.855	60.175	−412.882	−285.455	9.940
1600	57.024	127.622	86.477	65.832	−412.091	−276.986	9.043
1700	57.929	131.106	89.000	71.579	−411.280	−268.566	8.252
1800	58.831	134.443	91.433	77.417	−410.456	−260.195	7.551
1900	59.730	137.647	93.781	83.345	−409.624	−251.870	6.924
2000	60.626	140.734	96.052	89.363	−408.791	−243.589	6.362
2100	61.526	143.714	98.251	95.471	−407.960	−235.349	5.854
2200	62.413	146.596	100.384	101.668	−407.140	−227.148	5.393
2210.000	62.501	146.880	100.593	102.293	--- CRYSTAL <---> LIQUID ---		
2300	63.306	149.391	102.454	107.954	−406.337	−218.985	4.973
2400	64.199	152.104	104.466	114.329	−405.562	−210.856	4.589
2500	65.091	154.743	106.425	120.794	−404.831	−202.759	4.236
2600	65.982	157.313	108.333	127.347	−404.165	−194.689	3.911
2700	66.871	159.820	110.194	133.990	−403.604	−186.644	3.611
2800	67.760	162.268	112.010	140.722	−429.560	−178.131	3.323

PREVIOUS. CURRENT: December 1973

$S°(298.15\ K) = [83.233]\ J·K^{-1}·mol^{-1}$ $\Delta_f H°(298.15\ K) = [-336.743]\ kJ·mol^{-1}$
$T_{fus} = 2210 \pm 15\ K$ $\Delta_{fus}H° = 85.354 \pm 20.9\ kJ·mol^{-1}$

Enthalpy of Formation

$\Delta_f H°$(NbO, l, 298.15 K) is calculated from $\Delta_f H°$(NbO, cr, 298.15K) by adding $\Delta_{fus}H°$ and the difference in enthalpy, $H°(2210\ K) - H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

There is no data reported in the literature concerning the heat capacity or enthalpy of NbO(l). We estimate a constant value of $C_p° = 15.0$ cal·K^{-1}·mol^{-1} for the liquid phase. A glass transition is also assumed at 1500 K, so as to insure the proper thermodynamic relationship between the crystal values and extrapolated liquid values. At temperatures below 1500 K, $C_p°$ values of the crystal are used. The entropy at 298.15 K is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

Elliott[1] reported the melting point of NbO(cr) as T_{fus} = 2222 K (IPTS–68). Measurements by Kolchin and Sumarokova[2] gave T_{fus} = 2212 K (IPTS–68). The vapor pressure study of NbO(cr, l) by Shchukarev *et al.*[3] gave T_{fus} = 2207 K. We adopt $T_{fus} = 2210 \pm 15$ K in order to maintain good consistency with the vapor pressure data. Since the crystal structure of NbO(cr) is a defect NaCl structure, we can estimate $\Delta_{fus}H° = 13.9$ kcal·mol^{-1} based on $\Delta_{fus}S° = 6.27$ cal·K^{-1}·mol^{-1} as observed for NaCl.[4] The data of Shchukarev *et al.*[3] are more consistent with $\Delta_{fus}H° = 20.4$ kcal·mol^{-1}, as determined from our analysis of the vapor pressures over NbO(cr, l).[4] We adopt $\Delta_{fus}H° = 20.4 \pm 5.0$ kcal·mol^{-1}. This leads to $\Delta_{fus}S° = 9.23$ cal·K^{-1}·mol^{-1} which is roughly 3 cal·K^{-1}·mol^{-1} greater than the NaCl value.[4]

Vaporization Data

The vapors over NbO(l) have been shown by Shchukarev *et al.*[3] to be NbO(g) and NbO_2(g). At 2300 K, the rates of the vapor pressures NbO_2(g):NbO(g) is 1.00:0.23.[3]

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[3]S. A. Shchukarev, G. A. Semenoo, and K. E. Frantseva, Russ. J. Inorg. Chem. **11**, 129 (1966).
[4]JANAF Thermochemical Tables: NaCl(cr), 9–30–64, NbO(g), 12–31–73.

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

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							
100							
200							
250							
298.15	41.112	83.233	83.233	0.	−336.743	−320.105	56.081
300	41.187	83.488	83.234	0.076	−336.740	−320.002	55.717
400	44.032	95.764	84.888	4.350	−336.459	−314.460	41.064
500	45.827	105.793	88.097	8.848	−336.056	−309.005	32.282
600	47.204	114.273	91.771	13.501	−335.595	−303.638	26.434
700	48.369	121.638	95.523	18.280	−335.099	−298.351	22.263
800	49.467	128.169	99.203	23.173	−334.573	−293.136	19.140
900	50.481	134.054	102.754	28.170	−334.017	−287.990	16.714
1000	51.467	139.424	106.156	33.268	−333.430	−282.907	14.778
1100	52.418	144.374	109.408	38.462	−332.810	−277.884	13.196
1200	53.359	148.975	112.516	43.751	−332.156	−272.920	11.880
1300	54.287	153.283	115.488	49.134	−331.464	−268.011	10.769
1400	55.208	157.340	118.334	54.608	−330.734	−263.157	9.819
1500	56.120	161.180	121.063	60.175	−329.970	−258.357	8.997
1500.000	56.120	161.180	121.063	60.175	GLASS <---> LIQUID		
1500.000	62.760	161.180	121.063	60.175	TRANSITION		
1600	62.760	165.231	123.699	66.451	−328.560	−253.629	8.280
1700	62.760	169.035	126.255	72.727	−327.221	−248.987	7.650
1800	62.760	172.623	128.732	79.003	−325.959	−244.422	7.093
1900	62.760	176.016	131.132	85.279	−324.779	−239.925	6.596
2000	62.760	179.235	133.458	91.555	−323.687	−235.487	6.150
2100	62.760	182.297	135.711	97.831	−322.689	−231.102	5.748
2200	62.760	185.217	137.895	104.107	−321.789	−226.762	5.384
2210.000	62.760	185.501	138.110	104.734	--- CRYSTAL <---> LIQUID ---		
2300	62.760	188.006	140.014	110.383	−320.997	−222.461	5.052
2400	62.760	190.677	142.070	116.659	−320.321	−218.192	4.749
2500	62.760	193.239	144.066	122.935	−319.778	−213.948	4.470
2600	62.760	195.701	146.004	129.211	−319.389	−209.723	4.213
2700	62.760	198.070	147.889	135.487	−319.195	−205.510	3.976
2800	62.760	200.352	149.722	141.763	−345.607	−200.815	3.746
2900	62.760	202.554	151.506	148.039	−344.657	−195.661	3.524
3000	62.760	204.682	153.244	154.315	−343.717	−190.539	3.318

PREVIOUS: CURRENT: December 1973

CRYSTAL-LIQUID

0 to 2210 K crystal
above 2210 K liquid

Refer to the individual tables for details.

Enthalpy Reference Temperature = T_r = 298.15 K

Standard State Pressure = p° = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
0							
100							
200							
250							
298.15	41.112	46.024	46.024	0.	−419.655	−391.923	68.663
300	41.187	46.279	46.025	0.076	−419.652	−391.751	68.210
400	44.032	58.555	47.679	4.350	−419.371	−382.488	49.948
500	45.827	68.584	50.888	8.848	−418.968	−373.313	39.000
600	47.204	77.064	54.562	13.501	−418.507	−364.224	31.709
700	48.369	84.429	58.314	18.280	−418.011	−355.216	26.507
800	49.467	90.960	61.994	23.173	−417.485	−346.281	22.610
900	50.481	96.845	65.545	28.170	−416.929	−337.414	19.583
1000	51.467	102.215	68.947	33.268	−416.342	−328.610	17.165
1100	52.418	107.165	72.199	38.462	−415.722	−319.866	15.189
1200	53.359	111.766	75.307	43.751	−415.068	−311.181	13.545
1300	54.287	116.074	78.279	49.134	−414.376	−302.551	12.157
1400	55.208	120.131	81.125	54.608	−413.646	−293.976	10.968
1500	56.117	123.971	83.855	60.175	−412.882	−285.455	9.940
1600	57.024	127.622	86.477	65.832	−412.091	−276.986	9.043
1700	57.929	131.106	89.000	71.579	−411.280	−268.566	8.252
1800	58.831	134.443	91.433	77.417	−410.456	−260.195	7.551
1900	59.730	137.647	93.781	83.345	−409.624	−251.870	6.924
2000	60.626	140.734	96.052	89.363	−408.791	−243.589	6.362
2100	61.526	143.714	98.251	95.471	−407.960	−235.349	5.854
2200	62.413	146.596	100.384	101.668	−407.140	−227.148	5.393
2210.000	62.501	146.880	100.593	102.293	CRYSTAL <--> LIQUID TRANSITION		
2210.000	62.760	185.501	100.593	187.646			
2300	62.760	188.006	103.965	193.295	−320.997	−222.461	5.052
2400	62.760	190.677	107.523	199.571	−320.321	−218.192	4.749
2500	62.760	193.239	110.901	205.847	−319.778	−213.948	4.470
2600	62.760	195.701	114.115	212.123	−319.389	−209.723	4.213
2700	62.760	198.070	117.181	218.399	−319.195	−205.510	3.976
2800	62.760	200.352	120.111	224.675	−345.607	−200.815	3.746
2900	62.760	202.554	122.916	230.951	−344.657	−195.661	3.524
3000	62.760	204.682	125.606	237.227	−343.717	−190.539	3.318

PREVIOUS:

CURRENT December 1973

$S°(298.15\ K) = 238.976 \pm 3.56\ J\cdot K^{-1}\cdot mol^{-1}$

$\Delta_f H°(0\ K) = 199.54 \pm 20.9\ kJ\cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = 198.74 \pm 20.9\ kJ\cdot mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$X[^4\Sigma^-]$	0	4
$[^4\Pi]$	15000	8
$[^4\Sigma^-]$	21316.2	4

$\omega_e = 989.03\ cm^{-1}$ $\omega_e x_e = 3.83\ cm^{-1}$ $\sigma = 1$
$B_e = 0.432\ cm^{-1}$ $\alpha_e = 2.1 \times 10^{-3}\ cm^{-1}$ $r_e = 1.691$ Å

Enthalpy of Formation

Using the adopted vibrational constants [ω_e and $\omega_e x_e$], we calculate $D_0^\circ = 7.855$ eV as the dissociation energy of NbO(g) based on the linear Birge–Sponer extrapolation of the ground state. Applying a correction for the ionicity in the Nb–O bond as suggested by Hildenbrand and Murad,[1] we recalculate $D_0^\circ = 8.032$ eV. This latter value corresponds to $\Delta_f H°$(NbO, g, 298.15 K) = 48.03 kcal·mol^{-1}, assuming dissociation to normal atoms, while the former yields 52.11 kcal·mol^{-1}.

Shchukarev *et al.*[2,3] have investigated mass spectrometrically the composition of the vapors over NbO(cr, l) and NbO_2(cr, l). In their first work,[2] the authors reported that, besides NbO sublimation at 1773–1923 K, the reaction 2 NbO(cr) = Nb(cr) + NbO_2(g) occurs. A 2nd law $\Delta_{sub}H° = 138 \pm 3$ kcal·mol^{-1} was reported for the range 1773–1923 K. Using auxiliary data,[5] we calculate $\Delta_f H°$(NbO, g, 298.15 K) = 47.2 ± 3.0 kcal·mol^{-1}, assuming the $\Delta_{sub}H°$ reported value refers to 1900 K.

Shchukarev *et al.*[3] measured the vapor pressures of NbO and NbO_2(cr, l) and NbO_2(cr, l) by the effusion method coupled with a mass spectrometer. The results are summarized in the following table.

Reaction	T/K	$\Delta_f H°$(298.15 K), kcal·mol^{-1} 2nd law	3rd law	Drift cal·K^{-1}·mol^{-1}	$\Delta_f H°$(298.15 K), kcal·mol^{-1} 2nd law	3rd law
NbO(cr) = NbO(g)	1773–2210	148.0	147.5	−0.24	47.7	47.2
NbO(l) = NbO(g)	2210–2473	128.1	128.0	−0.04	47.6	47.5

We adopt $\Delta_f H°(298.15\ K) = 47.5 \pm 5.0$ kcal·mol^{-1} for NbO(g). The adopted value is an average value based on the 2nd and 3rd law results tabulated above. It is interesting to note that the adjusted Birge–Sponer result shows excellent agreement with the adopted $\Delta_f H°$(298.15 K). The adopted $\Delta_f H°$(298.15 K) leads to a dissociation energy $D_0^\circ = 8.05$ eV.

Heat Capacity and Entropy

The spectroscopic work involving NbO(g) has been reviewed and referenced by Rosen.[4] The adopted vibrational and rotational constants as well as the electronic levels are those tabulated by Rosen.[4] As indicated in Rosen,[4] the data suggest a $^4\Sigma^-$ ground state as in VO(g).[5] However, a possible ground state $^2\Delta$ as in TaO(g)[5] is not definitely excluded. The recent reviews by Cheetham and Barrow[6] and Weltner[7] favor a $^2\Delta$ ground state. Using a $^2\Delta$ ground state and $^2\Delta^{-2}\Delta$ transition at 21316.2 cm^{-1} produces the same thermodynamic functions as does a $^4\Sigma^-$ ground state and a $^4\Sigma$–$^4\Sigma$ transition at 21316.2 cm^{-1}. Green *et al.*[9] studied the infrared absorption spectra of isotopic NbO isolated in an Ar matrix. Green *et al.*[9] reported that a partial analysis of the observed bands supported the assignment of a $^4\Sigma^-$ electronic ground state for NbO.

The Gibbs energy functions used here are approximately 0.85 cal·K^{-1}·mol^{-1} at 298 K and 2.90 cal·K^{-1}·mol^{-1} at 3000 K lower than those proposed by Brewer and Rosenblatt.[8] The difference arises from the fact that Brewer and Rosenblatt[8] approximated the NbO electronic levels by using Nb^{++} electronic levels (which included low lying levels) whereas we have used the observed NbO electronic levels.

References

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[9] D. W. Green, W. Korfmacher and D. M. Gruen, J. Chem. Phys. 58, 404 (1973).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

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	−8.781	199.541	199.541	INFINITE
100	29.106	206.753	265.477	−5.872	200.216	189.462	−98.965
200	29.467	226.986	241.744	−2.952	199.584	178.910	−46.727
250	30.057	233.620	239.478	−1.464	199.157	173.791	−36.312
298.15	30.788	238.976	238.976	0.	198.740	168.943	−29.598
300	30.818	239.166	238.976	0.057	198.724	168.758	−29.383
350	31.614	243.977	239.354	1.618	198.301	163.798	−24.445
400	32.364	248.248	240.204	3.218	197.891	158.897	−20.750
450	33.033	252.099	241.315	4.853	197.492	154.047	−17.881
500	33.613	255.610	242.572	6.519	197.099	149.241	−15.591
600	34.531	261.824	245.276	9.929	196.316	139.742	−12.166
700	35.197	267.200	248.033	13.417	195.521	130.376	−9.729
800	35.687	271.934	250.730	16.963	194.700	121.125	−7.909
900	36.054	276.159	253.325	20.550	193.847	111 979	−6.499
1000	36.336	279.973	255.803	24.171	192.956	102.930	−5.377
1100	36.557	283.447	258.160	27.816	192.026	93.972	−4.462
1200	36.735	286.636	260.402	31.481	191.056	85.101	−3.704
1300	36.880	289.582	262.535	35.161	190.047	76.312	−3 066
1400	37.002	292.320	264.566	38.856	188.997	67.602	−2.522
1500	37.106	294.876	266.502	42.561	187.900	58.969	−2.053
1600	37.196	297.274	268.351	46.277	186.749	50.411	−1.646
1700	37.277	299.531	270.120	50.000	185.536	41.926	−1.288
1800	37.352	301.664	271.813	53.732	184.254	33.515	−0 973
1900	37.423	303.686	273.438	57 471	182.896	25.177	−0 692
2000	37.493	305.607	274.999	61.216	181.457	16.913	−0.442
2100	37.564	307.438	276.500	64.969	179.933	8.723	−0.217
2200	37.638	309.187	277.947	68.729	178.316	0.608	−0.014
2300	37.717	310.862	279.342	72.497	176.601	−7.432	0.169
2400	37.802	312.469	280.689	76.273	174.776	−15.394	0.335
2500	37.895	314.014	281.991	80.057	172.828	−23.279	0.486
2600	37.997	315.502	283.251	83.852	170.735	−31.082	0.624
2700	38.108	316.938	284.473	87.657	168.458	−38.802	0.751
2800	38.230	318.326	285.657	91.474	139.587	−45.948	0.857
2900	38.362	319.670	286.807	95.303	138.091	−52.549	0.947
3000	38.506	320.973	287.924	99.147	136.598	−59.097	1.029
3100	38.660	322.238	289.011	103.005	135.111	−65.595	1.105
3200	38.825	323.468	290.068	106.879	133.631	−72.046	1.176
3300	39.000	324.665	291.099	110.770	132.160	−78.451	1.242
3400	39.185	325.832	292.103	114.679	130.698	−84.811	1.303
3500	39.380	326.971	293.083	118.607	129.247	−91.128	1.360
3600	39.583	328.083	294.040	122.556	127.808	−97.404	1.413
3700	39.794	329.171	294.975	126.524	126.383	−103.641	1.463
3800	40.012	330.235	295.889	130.515	124.972	−109.838	1.510
3900	40.236	331.277	296.783	134.527	123.576	−115.999	1.554
4000	40.466	332.299	297.658	138.562	122.196	−122.125	1.595
4100	40.700	333.301	298.515	142.620	120.833	−128.216	1.633
4200	40.937	334.284	299.355	146.702	119.487	−134.274	1.670
4300	41.177	335.250	300.179	150.808	118.158	−140.300	1.704
4400	41.418	336.200	300.987	154.938	116.848	−146.296	1.737
4500	41.661	337.133	301.780	159.091	115.556	−152.262	1 767
4600	41.903	338.052	302.558	163.270	114.281	−158.199	1.796
4700	42.144	338.955	303.323	167.472	113.025	−164.109	1.824
4800	42.384	339 845	304.075	171.699	111.787	−169.992	1.850
4900	42.622	340.722	304.814	175 949	110.566	−175.850	1.875
5000	42.856	341.585	305.540	180.223	109.363	−181.683	1.898
5100	43.087	342.436	306.256	184.520	108.175	−187.492	1.920
5200	43.313	343.275	306.959	188.840	−583.668	−183.969	1.848
5300	43.535	344.102	307.652	193.182	−585.156	−176.268	1.737
5400	43.752	344.918	308.335	197.547	−586.603	−168.543	1.630
5500	43.963	345.722	309.007	201.933	−588.110	−160.788	1.527
5600	44.168	346.516	309.670	206.339	−589.633	−153.004	1.427
5700	44.366	347.300	310.323	210.766	−591.173	−145.194	1.331
5800	44.559	348.073	310.968	215.212	−592.731	−137.356	1.237
5900	44.744	348.837	311.603	219.677	−594.309	−129.492	1.146
6000	44.922	349.590	312.230	224.161	−595.909	−121.600	1.059

PREVIOUS: December 1973 (1 atm) CURRENT. December 1973 (1 bar)

$S°(298.15\ K) = 54.506 \pm 0.29\ J·K^{-1}·mol^{-1}$
$T_{trs1} = 1090 \pm 20\ K$
$T_{trs2} = 1200\ K$
$T_{fus} = 2175 \pm 15\ K$

$\Delta_f H°(0\ K) = -790.31 \pm 8.4\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = -794.96 \pm 8.4\ kJ·mol^{-1}$
$\Delta_{trs1} H° = 3.423\ kJ·mol^{-1}$
$\Delta_{trs2} H° = 0.000\ kJ·mol^{-1}$
$\Delta_{fus} H° = 92.048 \pm 20.9\ kJ·mol^{-1}$

Enthalpy of Formation

There are three oxygen bomb calorimetric studies for NbO_2(cr). As with NbO(cr), the combustion results must be interpreted inlight of impure samples, possible incomplete combustion, and possible nonstoichiometry. The following $\Delta_c H°$ results have been reported for the oxygen combustion of one mole of NbO_2(cr) to yield Nb_2O_5(cr). 37.0 ± 0.4 kcal·mol^{-1} (291 K) by Morozova and Getskina,[1] 37.6 ± 2.6 kcal·mol^{-1} (298 K) by Kusenko and Gel'd,[2] and 36.67 ± 0.10 kcal·mol^{-1} (298 K) by Mah.[3] Using the value $\Delta_f H°(298.15\ K) = 37.0 \pm 2.0$ kcal·mol^{-1} and JANAF auxiliary data,[4] we calculate and adopt $\Delta_f H°(NbO_2, cr, 298.15\ K) = -190.0 \pm 2.0$ kcal mol^{-1}.

There are numerous equilibrium studies involving NbO_2. Early work involved the reduction of niobium oxides with hydrogen by Grube *et al.*,[5] Sue,[6] and Schaefer and Breil,[7] and the carbon reduction of Nb_2O_5 by Sue.[8] The more recent emf equilbrium studies are analyzed and tabulated in the following table.

Source	T/K	Reaction	$\Delta_f H°(298.15\ K)$, kcal·mol^{-1} 2nd law	3rd law	Drift cal·K^{-1}·mol^{-1}	$\Delta_f H°(298.15\ K)$ kcal·mol^{-1}
[9]	1673–1823	$NbO_2(cr)+H_2(g)=NbO(cr)+H_2O(g)$	36.35	32.30	−2.3	−190.4
[10]	1100–1300	$NbO_2(cr)+Nb(cr)=2\ NbO(cr)$	−11.96	−9.59	2.0	−187.8
[11]	1074–1175	$Nb_2O_5(cr)+C(cr)=2\ NbO_2(cr)+CO(g)$	38.43	45.87	6.6	−190.9
[12]	1177–1361	$NbO(cr)+1/3\ Cr_2O_3(cr)=NbO_2(cr)+2/3\ Cr(cr)$	2.32	1.78	−0.4	−188.9

Heat Capacity and Entropy

King (53–296 K)[13] measured the heat capacity of NbO_2(cr). Using the combination of Debye and Einstein functions suggested by King,[13] we calculate $S°(51\ K) = 0.616$ cal·K^{-1}·mol^{-1} and $H°(51\ K)-H°(0\ K) = 23$ cal·K^{-1}·mol^{-1}. The enthalpy data of Gel'd and Kusenko,[14] and King and Christensen,[15] indicated a transition in the region 1000–1200 K. We adopt the reported enthalpy equations of King and Christensen[15] for the ranges 1090–1200 K and 1200–1800 K. The latter equation is extrapolated to T_{fus}. For the region 298–1090 K, we use a five term polynomial to fit the enthalpy data of King and Christensen[15] with constraints to join smoothly with the enthalpy derived from the King data:[13] the deviations are +0.34 to −0.67% in this range 298–1090 K. In the same range, the Gel'd and Kusenko data[14] lies approximately 2–3% higher; for $T > 1200$ K, it is 0.6–2.5% high.

Phase Data

Brauer[16] reported a homogeneity range of $x = 1.95$ to 2.05 for NbO_2. A recent study by Janninck and Whitmore,[17] using isopiestic reduction techniques at 1373 K, reported $x = 1.9975$ to 2.003.

Brauer,[16] Magneli *et al.*,[18] Terao,[19] and Marınder[20] have shown that at room temperature NbO_2 has a deformed rutile structure. NbO_2 is similar to V_2O_4 in terms of crystal structure.[21]

TransitionData

Electric conductivity and thermoelectric power measurements and a DTA and x-ray diffraction study indicated a phase transition in the region 1068–1173 K.[17,21,22] In this region, the structure of NbO_2 transforms from a deformed rutile to a rutile structure. The evidence suggested that the transition is not sharp but is actually spread over at least 50°.[21]

The enthalpy data of King and Christensen[15] and Gel'd and Kusenko[14] are consistent with the above interpretation. We treat this transition as first order with $T_{trs1} = 1090 \pm 20$ K and add an artificial transition $T_{trs2} = 1200$ K as in King and Christensen.[15] This combination reduces the reported enthalpy data.[15] The value $\Delta_{trs1} H° = 0.818$ kcal·mol^{-1} is calculated as the difference between the enthalpies of the two "phases" at 1090 K associated with the transition at T_{trs1}.

Fusion Data

Refer to the liquid table for details.

Sublimation Data

$\Delta_{sub} H°(298.15\ K) = 142.1 \pm 5.0$ kcal·mol^{-1} is calculated as the $\Delta_f H°(298.15\ K)$ differences for NbO_2(g) and NbO_2(cr).

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[4] JANAF Thermochemical Tables: Nb_2O_5(cr), 12-31-72, NbO(cr), 12-31-73.

Continued on page 1693

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

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	−9.271	−790.308	−790.308	INFINITE
100	21.143	11.275	96.297	−8.502	−793.224	−775.765	405.218
200	44.918	33.967	59.417	−5.090	−794.821	−757.542	197.850
298.15	57.452	54.506	54.506	0.	−794.960	−739.175	129.500
300	57.605	54.862	54.507	0.106	−794.954	−738.829	128.642
400	63.547	72.327	56.848	6.191	−794.348	−720.199	94.048
500	67.739	86.967	61.447	12.760	−793.403	−701.766	73.313
600	71.651	99.665	66.781	19.730	−792.205	−683.547	59.508
700	75.555	111.003	72.302	27.090	−790.755	−665.549	49.664
800	79.496	121.348	77.795	34.843	−789.037	−647.776	42.295
900	83.479	130.941	83.173	42.991	−787.033	−630.236	36.578
1000	87.500	139.945	88.405	51.540	−784.726	−612.934	32.016
1090.000	91.144	147.640	92.980	59.579	I <--> II		
1090.000	92.885	150.780	92.980	63.001	TRANSITION		
1100	92.885	151.628	93.510	63.930	−778.665	−595.911	28.297
1200	92.885	159.710	98.694	73.219	−775.786	−579.425	25.222
1200.000	92.885	159.710	98.694	73.219	II <--> III		
1200.000	83.052	159.710	98.694	73.219	TRANSITION		
1300	83.052	166.358	103.647	81.524	−773.962	−563.136	22.627
1400	83.052	172.513	108.349	89.829	−772.208	−546.984	20.408
1500	83.052	178.243	112.820	98.135	−770.526	−530.956	18.490
1600	83.052	183.603	117.078	106.440	−768.921	−515.038	16.814
1700	83.052	188.638	121.141	114.745	−767.398	−499.217	15.339
1800	83.052	193.385	125.024	123.050	−765.965	−483.484	14.030
1900	83.052	197.875	128.741	131.355	−764.626	−467.827	12.861
2000	83.052	202.135	132.305	139.661	−763.386	−452.239	11.811
2100	83.052	206.188	135.728	147.966	−762.251	−436.710	10.863
2175.000	83.052	209.102	138.208	154.195	----- III <--> LIQUID -----		
2200	83.052	210.051	139.019	156.271	−761.226	−421.232	10.001
2300	83.052	213.743	142.188	164.576	−760.320	−405.799	9.216
2400	83.052	217.278	145.244	172.882	−759.541	−390.402	8.497
2500	83.052	220.668	148.193	181.187	−758.906	−375.035	7.836
2600	83.052	223.925	151.044	189.492	−758.437	−359.690	7.226
2700	83.052	227.060	153.802	197.797	−758.172	−344.359	6.662
2800	83.052	230.080	156.472	206.103	−784.523	−328.549	6.129

PREVIOUS: CURRENT: December 1973

$S°(298.15\ K) = [92{,}835]\ J·K^{-1}·mol^{-1}$
$T_{fus} = 2175 \pm 15\ K$

$\Delta_f H°(298.15\ K) = [-710.872]\ kJ·mol^{-1}$
$\Delta_{fus} H° = 92.048 \pm 20.9\ kJ·mol^{-1}$

Enthalpy of Formation

$\Delta_f H°(NbO_2, l, 298.15\ K)$ is calculated from $\Delta_f H°(NbO_2, cr, 298.15\ K)$ by adding $\Delta_{fus} H°$ and the difference in enthalpy, $H°(2175\ K) - H(298.15\ K)$, between the crystal and the liquid.

Heat Capacity and Entropy

There is no data reported in the literature concerning the heat capacity or enthalpy of NbO_2(l). We estimate a constant value of $C_p° = 7.5$ cal·K^{-1}·g–atom^{-1} or 22.5 cal·K^{-1}·mol^{-1} for the liquid phase. A glass transition is assumed at 1000 K below which the $C_p°$ values of the crystal are used. The entropy at 298.15 K is calculated in a manner analogous to that used in calculating the enthalpy of formation.

Fusion Data

Elliott[1] reported the melting point of NbO_2(cr) as $T_{fus} = 2191$ K (IPTS–68) and stated that NbO_2(cr) melts without decomposition. The vapor pressure study on NbO_2(cr, l) by Shchukarev *et al.*[2] gave $T_{fus} = 2173$ K (IPTS–68) with congruent melting. We adopt $T_{fus} = 2175 \pm 15$ K in order to maintain good consistency with the vapor pressure data. A value of $T_{fus} = 2357$ K reported by Kolchin and Sumarokova[3] appears too high.

The vapor pressure data of Shchukarev *et al.*[2] suggests $\Delta_{fus} H° = 22.0$ kcal·mol^{-1} which we adopt. This leads to $\Delta_{fus} S° = 10.11$ cal·K^{-1}·mol^{-1}.

Vaporization Data

The vapors over NbO_2(l) have been shown by Shchukarev *et al.*[2] to be NbO(g), NbO_2(g), and O(g). At 2300 K, the ratio of the vapor pressures NbO_2(g):NbO(g) is 1.00:0.07.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

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							
100							
200							
298.15	*57.450*	*92.835*	*92.835*	0.	−710.872	−666.514	116.771
300	57.605	93.191	92.836	0.106	−710.865	−666.239	116.003
400	63.547	110.656	95.177	6.191	−710.259	−651.442	85.070
500	67.739	125.296	99.776	12.760	−709.314	−636.842	66.530
600	71.651	137.993	105.109	19.730	−708.116	−622.456	54.190
700	75.555	149.331	110.631	27.090	−706.667	−608.290	45.391
800	79.496	159.677	116.124	34.843	−704.949	−594.351	38.807
900	83.479	169.270	121.502	42.991	−702.945	−580.643	33.700
1000	87.500	178.273	126.733	51.540	−700.637	−567.175	29.626
1000.000	87.500	178.273	126.733	51.540	GLASS <---> LIQUID TRANSITION		
1000.000	*94.140*	178.273	126.733	51.540			
1100	94.140	187.246	131.833	60.954	−697.553	−553.978	26.306
1200	94.140	195.437	136.797	70.368	−694.548	−541.059	23.552
1300	94.140	202.972	141.602	79.782	−691.616	−528.388	21.231
1400	94.140	209.949	146.237	89.196	−688.753	−515.940	19.250
1500	94.140	216.444	150.704	98.610	−685.962	−503.694	17.540
1600	94.140	222.520	155.005	108.024	−683.248	−491.632	16.050
1700	94.140	228.227	159.146	117.438	−680.617	−479.737	14.741
1800	94.140	233.608	163.134	126.852	−678.075	−467.994	13.581
1900	94.140	238.698	166.979	136.266	−675.627	−456.390	12.547
2000	94.140	243.526	170.686	145.680	−673.278	−444.913	11.620
2100	94.140	248.119	174.265	155.094	−671.034	−433.550	10.784
2175.000	94.140	251.423	176.869	162.154	----- III <---> LIQUID -----		
2200	*94.140*	252.499	177.722	164.508	−668.901	−422.291	10.026
2300	94.140	256.683	181.065	173.922	−666.886	−411.128	9.337
2400	94.140	260.690	184.300	183.336	−664.998	−400.049	8.707
2500	94.140	264.533	187.433	192.750	−663.254	−389.046	8.129
2600	94.140	268.225	190.470	202.164	−661.676	−378.109	7.596
2700	94.140	271.778	193.416	211.578	−660.303	−367.229	7.104
2800	94.140	275.202	196.276	220.992	−685.546	−355.912	6.640
2900	94.140	278.505	199.055	230.406	−683.437	−344.177	6.199
3000	94.140	281.697	201.757	239.820	−681.347	−332.514	5.790

PREVIOUS· CURRENT: December 1973

CRYSTAL(I–II–III)–LIQUID

0	to	1090 K	crystal, I
1090	to	1200 K	crystal, II
1200	to	2175 K	crystal, III
above		2175 K	liquid

Refer to the individual tables for details.

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = p° = 0.1 MPa

	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
T/K	C_p°	S°	$-[G^\circ - H^\circ(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
0	0.	0.	INFINITE	−9.271	−790.308	−790.308	INFINITE
100	21.143	11.275	96.297	−8.502	−793.224	−775.765	405.218
200	44.918	33 967	59.417	−5.090	−794.821	−757.542	197.850
298.15	57.452	54.506	54.506	0.	−794.960	−739.175	129.500
300	57.605	54.862	54.507	0.106	−794.954	−738.829	128.642
400	63.547	72.327	56.848	6.191	−794.348	−720.199	94.048
500	67.739	86.967	61.447	12.760	−793.403	−701.766	73.313
600	71.651	99.665	66.781	19.730	−792.205	−683.547	59.508
700	75.555	111.003	72.302	27.090	−790.755	−665.549	49.664
800	79.496	121.348	77.795	34.843	−789.037	−647.776	42.295
900	83.479	130.941	83.173	42.991	−787.033	−630.236	36.578
1000	87.500	139.945	88.405	51.540	−784.726	−612.934	32.016
1090.000	91.144	147.640	92.980	59.579	I <--> II		
1090.000	92.885	150.780	92.980	63.001	TRANSITION		
1100	92.885	151.628	93.510	63.930	−778.665	−595.911	28.297
1200	92.885	159.710	98.694	73.219	−775.786	−579.425	25.222
1200.000	92.885	159.710	98.694	73.219	II <--> III		
1200.000	83.052	159.710	98.694	73.219	TRANSITION		
1300	83.052	166.358	103.647	81.524	−773.962	−563.136	22.627
1400	83.052	172.513	108.349	89.829	−772.208	−546.984	20.408
1500	83.052	178.243	112.820	98.135	−770.526	−530.956	18.490
1600	83.052	183.603	117.078	106.440	−768.921	−515.038	16.814
1700	83.052	188.638	121.141	114.745	−767.398	−499.217	15.339
1800	83.052	193.385	125.024	123.050	−765.965	−483.484	14.030
1900	83.052	197.875	128.741	131.355	−764.626	−467.827	12.861
2000	83.052	202.135	132.305	139.661	−763.386	−452.239	11.811
2100	83.052	206.188	135.728	147.966	−762.251	−436.710	10.863
2175.000	83.052	209.102	138.208	154.195	III <--> LIQUID		
2175.000	94.140	251.423	138.208	246.243	TRANSITION		
2200	94.140	252.499	139.500	248.596	−668.901	−422.291	10.026
2300	94.140	256.683	144.505	258.010	−666.886	−411.128	9.337
2400	94.140	260.690	149.263	267.424	−664.998	−400.049	8 707
2500	94.140	264.533	153.798	276.838	−663.254	−389.046	8.129
2600	94.140	268.225	158.128	286.252	−661.676	−378.109	7.596
2700	94.140	271.778	162.272	295.666	−660.303	−367.229	7.104
2800	94.140	275.202	166.245	305.080	−685.546	−355.912	6.640
2900	94.140	278.505	170.059	314.494	−683 437	−344.177	6.199
3000	94.140	281.697	173.727	323.908	−681.347	−332.514	5.790

PREVIOUS CURRENT: December 1973

$S°(298.15\ K) = [272.921 \pm 8.4]\ J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K) = -197.33 \pm 20.9\ kJ·mol^{-1}$

$\Delta_f H°(298.15\ K) = -200.00 \pm 20.9\ kJ·mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[970](1)
[300](1)
[930](1)

Ground State Quantum Weight: [2] σ = [2]
Point Group: [C_{2v}]
Bond Distance: Nb–O = [1.691] Å
Bond Angle: O–Nb–O = [110]°
Product of the Moments of Inertia: $I_A I_B I_C$ = [5.274350 × 10^{-115}] $g^3·cm^6$

Enthalpy of Formation

Shchukarev *et al.*[1-4] measured the vapor pressures of NbO and NbO_2 over NbO(cr, l) and NbO_2(cr, l) by the effusion method coupled with a mass spectrometer. An analysis of the reported smoothed results is presented in the following table.[4]

Reaction	T/K	$\Delta_r H°$(298.15 K), kcal·mol^{-1} 2nd law	3rd law	Drift cal·K^{-1}·mol^{-1}	$\Delta_f H°$(298.15 K), kcal·mol^{-1} 2nd law	3rd law
NbO_2(cr) = NbO_2(g)	1773–2175	142.0	143.4	0.69	−48.0	−46.6
NbO_2(l) = NbO_2(g)	2175–2473	124.2	123.7	−0.22	−46.8	−46.3
2 NbO(cr) = NbO_2(g) + Nb(cr)	1773–2210	147.8	149.9	1.03	−52.8	−50.7
2 NbO(l) = NbO_2(g) + Nb(cr)	2210–2473	119.7	111.1	−3.73	−41.3	−49.9

We adopt $\Delta_f H°(NbO_2, g, 298.15\ K) = -47.8 \pm 5.0$ kcal·mol^{-1}. This value is an average value of the 2nd and 3rd law results for the sublimation and vaporization of NbO_2. This adopted $\Delta_f H°$(298.15 K) value leads to $D_0°$ = 14.73 eV for the process $NbO_2(g) = Nb(g) + 2\ O(g)$. The $\Delta_{at} H°$(0 K) value is 1.83 times as great as the dissociation energy of NbO(g) ($D_0°$=8.05 eV).[2]

The earlier less complete studies by Shchukarev *et al.*[1-3] are in fair agreement with the above conclusions. Using a platinum strip to vaporize NbO_2(cr) in a mass spectrometer at temperatures of 1500 to 1880 K, Shchukarev *et al.*[1] reported a 2nd law sublimation heat, $\Delta_{sub} H°(1700\ K) = 142 \pm 3$ kcal·mol^{-1}. Using auxiliary data,[6] we calculate $\Delta_f H°(NbO_2, g, 298.15\ K) = -38.8$ kcal·mol^{-1}. The mass spectrometric investigation of the NbO(cr) evaporation by Shchukarev *et al.*[2] led to a reported value $\Delta_r H°(1800\ K) = 140 \pm 3$ kcal·mol^{-1} for the process 2 NbO(cr) = Nb(cr) + NbO_2(g). Using auxiliary data,[6] we calculate $\Delta_f H°(NbO_2, g, 298.15\ K) = -53.3$ kcal·mol^{-1}. NbO_2 pressures were obtained (1938–2122 K) by the differential effusion method using the radioactive tracer ^{95}Nb.[3] The pressures agree within 5% of those obtained in the more complete study.[4] Golubtsov *et al.*[5] also measured the vapor pressure of NbO_2(g) over NbO_2(cr) in the range 1489–1905 K by using labelled atoms in a Knudsen cell. The same authors also studied the dissociation of Nb_2O_5 in vacuo in the range 1432–1756 K, the process being $Nb_2O_5(cr) \rightarrow 2\ NbO_2(g) + 1/2\ O_2(g)$. These latter data[5] are not considered.

Heat Capacity and Entropy

The vibrational frequencies and geometry of NbO_2(g) are estimated based on existing and estimated data for related metal dioxides such as TiO_2(g), TaO_2(g), and WO_2(g).[6] The Nb–O bond distance is assumed to be the same as in NbO(g).[6] The ground state quantum weight of 2 is adopted so as to be consistent with TaO_2(g).[6] The principal moments of inertia are calculated as $I_A = 3.7181 \times 10^{-39}$, $I_B = 10.1954 \times 10^{-39}$, and $I_C = 13.9136 \times 10^{-39}$ g·cm^2.

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[6] JANAF Thermochemical Tables. NbO_2(cr), NbO(cr, g), Nb(cr), TaO_2(g) and TiO_2(g), 12–31–73; WO_2(g), 9–30–66.

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

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	−11.254	−197.325	−197.325	INFINITE
100	35.385	230.299	309.095	−7.880	−197.637	−202.080	105.556
200	39.819	256.260	276.805	−4.109	−198.875	−206.055	53.816
250	41.903	265.368	273.633	−2.066	−199.475	−207.779	43.413
298.15	43.907	272.921	272.921	0.	−199 995	−209.330	36.674
300	43.982	273.193	272.922	0.081	−200.014	−209.388	36.458
350	45.916	280.121	273.465	2.330	−200.488	−210.912	31.477
400	47.622	286.366	274.693	4.669	−200.905	−212.373	27.733
450	49.082	292.062	276.311	7.088	−201.280	−213.783	24.815
500	50.311	297.299	278.152	9.573	−201.625	−215.154	22.477
600	52.201	306.649	282.141	14.705	−202.266	−217.799	18.961
700	53.531	314.801	286.237	19.995	−202.886	−220.338	16.442
800	54.485	322.015	290.267	25.398	−203.517	−222.789	14.547
900	55 184	328.475	294.160	30.884	−204.176	−225.159	13.068
1000	55 708	334.317	297.888	36.429	−204.872	−227.453	11.881
1100	56.110	339.647	301.446	42.021	−205.609	−229.676	10.906
1200	56.424	344.543	304.836	47.649	−206.391	−231.829	10 091
1300	56 674	349.070	308.067	53.304	−207.217	−233.916	9.399
1400	56.875	353.277	311.147	58.982	−208.091	−235.937	8.803
1500	57.039	357.207	314.088	64.678	−209.018	−237.895	8.284
1600	57.175	360.893	316.900	70.388	−210.007	−239.788	7.828
1700	57.288	364.362	319.591	76.112	−211.067	−241.617	7.424
1800	57.384	367.640	322.170	81.846	−212.205	−243.382	7 063
1900	57 466	370.744	324.645	87.588	−213.428	−245.081	6.738
2000	57.536	373.694	327.025	93.338	−214.743	−246 713	6.443
2100	57.597	376.503	329.314	99.095	−216.157	−248.277	6.176
2200	57.649	379 183	331.521	104.857	−217.675	−249.771	5.930
2300	57.695	381.747	333.649	110.625	−219.306	−251.194	5.705
2400	57.736	384.203	335 705	116.396	−221.062	−252.544	5.496
2500	57.772	386.561	337.692	122.172	−222.956	−253.817	5.303
2600	57.804	388.827	339.616	127.951	−225.013	−255.012	5.123
2700	57.832	391.009	341.479	133.732	−227.272	−256.123	4.955
2800	57.858	393.113	343.286	139.517	−256.144	−256.662	4.788
2900	57.881	395.144	345.039	145.304	−257.662	−256.655	4.623
3000	57.902	397.106	346.742	151.093	−259 197	−256.593	4.468
3100	57.921	399.005	348.398	156.884	−260.749	−256.480	4.322
3200	57.938	400.845	350.008	162.677	−262.317	−256.318	4.184
3300	57.953	402.628	351.576	168.472	−263.901	−256.107	4.054
3400	57.967	404.358	353.103	174.268	−265.500	−255.846	3.931
3500	57.981	406.038	354.591	180.065	−267.113	−255.539	3.814
3600	57.992	407.672	356.043	185.864	−268.741	−255.185	3.703
3700	58.004	409.261	357.460	191.664	−270.382	−254.787	3.597
3800	58.014	410.808	358.844	197.465	−272.037	−254.342	3.496
3900	58.023	412.315	360.196	203.266	−273.705	−253.854	3.400
4000	58.032	413.784	361.517	209.069	−275.385	−253.325	3.308
4100	58.040	415.217	362.809	214.873	−277.077	−252.752	3.220
4200	58.047	416.616	364.074	220.677	−278.781	−252.138	3.136
4300	58.055	417.982	365.312	226.482	−280.497	−251.483	3.055
4400	58.061	419.317	366.524	232.288	−282.224	−250.789	2.977
4500	58.067	420.622	367.712	238.094	−283 963	−250.056	2.903
4600	58.073	421.898	368.876	243.901	−285.713	−249.283	2.831
4700	58.078	423.147	370.017	249.709	−287.476	−248.472	2.761
4800	58.083	424.370	371.137	255.517	−289.250	−247.623	2.695
4900	58.088	425.567	372.236	261.326	−291.036	−246.737	2.630
5000	58.092	426.741	373.314	267.135	−292.835	−245.815	2.568
5100	58.097	427.891	374.373	272.944	−294.647	−244.856	2.508
5200	58.101	429.020	375.413	278.754	−987.145	−234.553	2.356
5300	58 104	430.126	376.435	284.564	−989.316	−220.059	2.169
5400	58.108	431.212	377.439	290.375	−991.477	−205.529	1.988
5500	58.111	432.279	378.427	296.186	−993.725	−190.954	1.814
5600	58.114	433.326	379.398	301.997	−996.019	−176.337	1.645
5700	58.117	434.354	380.353	307.809	−998.359	−161.679	1.482
5800	58.120	435.365	381.293	313.621	−1000.745	−146.979	1.324
5900	58.123	436.359	382.218	319.433	−1003.180	−132.240	1.171
6000	58.126	437.336	383.128	325.245	−1005.664	−117.456	1.023

PREVIOUS. December 1973 (1 atm) CURRENT: December 1973 (1 bar)

$S°(298.15\ K) = 137.30 \pm 1.3\ J·K^{-1}·mol^{-1}$
$T_{fus} = 1785 \pm 30\ K$

$\Delta_f H°(0\ K) = -1889.616 \pm 4.2\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = -1899.536 \pm 4.2\ kJ·mol^{-1}$
$\Delta_{fus} H° = 104.265 \pm 2.1\ kJ·mol^{-1}$

Enthalpy of Formation

The $\Delta_f H°(Nb_2O_5, cr, 298.15\ K)$ investigations suffer from uncertainties concerning the polymorphic state of the samples employed and the oftentimes incomplete impurity analysis of the samples.[1] There is considerable scatter in the following tabulation for the enthalpy of formation values, all of which are based on enthalpy of combustion studies.

Source	Nb(cr) purity, %	% completion*	$\Delta_f H°(298.15\ K)$ kcal·mol^{-1}
[2]			−442.8
[3]	98.8	96.34–96.94	−459.9 ± 0.7**
[4]	99.69	97.63–99.38	−454.0 ± 0.6**
[5]			−472.6 ± 1.0
[6]	99.49		−454.8 ± 0.8
[7]			−458.6 ± 5.0
[8]	99.01	99.1–99.33	−455.1 ± 0.5
[9]	99.45	98.78–100	−454.4 ± 1.6
[10]	98.47–99.35	99.48–99.96	−453.5 ± 0.4
[11]	98.47–99.35	99.48–99.96	−453.5 ± 0.4
[12]			−456.9

* Percent completion refers to extent of reaction 2 Nb(cr) + 2.5 O_2(g) = Nb_2O_5(cr).
** Values adjusted by Kubaschewski and Catterall[13] to more satisfactorily correct for incomplete reaction.

The value chosen for $\Delta_f H°(Nb_2O_5, cr, 298.15\ K)$ is 454.0 ± 1 kcal·mol^{-1}. This value is representative of the work by Humphrey,[4] Kornilov *et al.*,[10, 11] Huber *et al.*,[9] Kusenko and Gel'd[8] and Morozova and Stolyarova.[6] These works have discussed sample purity and have percentage conversions of Nb(cr) to Nb_2O_5(cr) of the order of 97% or better. Based on the discussion by Reisman and Holtzberg,[1] this $\Delta_f H°(298.15\ K)$ value is for the high temperature α–phase of Nb_2O_5(cr). The heat capacity and enthalpy work, also dealing with Nb_2O_5(cr, α), indicated no phase changes for 53–297 K and 381–1785 K.[14, 16]

$\Delta_f G°$ values for Nb_2O_5(cr) in the range 1050 1300 K were calculated from measured emf values in an oxygen concentration cell and the known $\Delta_f G°$ values of Cr_2O_3.[17] The reported smoothed $\Delta_f G°$ values were treated by a 3rd law analysis, yielding $\Delta_f H°(Nb_2O_5, cr, 298.15\ K) = 451.6$ kcal·mol^{-1} with a drift equivalent to an entropy error of 4.8 cal·K^{-1}·mol^{-1}.

Heat Capacity and Entropy

King[14] measured the heat capacity of the high temperature α–phase Nb_2O_5 from 53.24 to 296.64 K and fitted the data (29 data points) with a combination of Debye and Einstein functions. These functions fit the data over the entire measured temperature range with a maximum deviation of 0.6%[14] and are used to calculate $S°(50\ K) = 2.42$ cal·K^{-1}·mol^{-1}.

Orr[15] using the same material as King,[14] measured the enthalpy from 381.4 to 1809.2 K. Gel'd and Kusenko[16] also measured the enthalpy from 461 to 1828 K. Combining these data[15 16] with a portion of the King data (a $C_p°$ fit, then integrated), a six term polynomial fit is used to represent the enthalpy data, yielding a deviation of 0.99% to +0.81% for the Orr data and 0.64% to + 1.10% for the Gel'd and Kusenko data. Two points (644 K, 734 K) of the Gel'd and Kusenko data are not used as they deviate from the polynomial fitted values by 2–3%. Entahlpy values corresponding to temperatures greater than 1750 K but less than T_{fus} are considered to be involved in premelting.[15] Enthalpy values for $1785 \le T \le 2300$ K are obtained by extrapolating the values obtained from the polynomial fit. The chosen heat capacity values are obtained by differentiating the enthalpy polynomial fit for the range 298–2300 K. For temperatures 50 298 K, the King data were fit to a six term polynomial.

The existing experimental data[14,15 16] did not indicate any transitions other than a crystal liquid transition. Lacking thermodynamic information for the other crystal phases of Nb_2O_5,[1] we assume that there is little difference in the heat capacity and enthalpy values for the various crystal phases. Thus the values tabulated here apply to all crystal Nb_2O_5 phases. The data for Ta_2O_5(cr) presented in these tables are treated in the same manner as discussed here so as to maintain consistency between Nb_2O_5(cr, I) and Ta_2O_5(cr, I).

Fusion Data

Refer to the liquid table for details.

References

[1] A. Reisman and F. Holtzberg, High Temp. Oxides 2, 217 (1970).
[2] W. Muthmann, L. Weiss, and R. Reidelbauch, Ann. Chem. 355, 67, 82 (1907).
[3] G. Becker and W. A. Roth, Z. Physik. Chem. 167A, 16 (1933).

Continued on page 1693

Enthalpy Reference Temperature = T_r = 298.15 K *Standard State Pressure = $p°$ = 0.1 MPa*

	J·K^{-1}·mol^{-1}			kJ·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	0.	0.	INFINITE	−22.287	−1889.634	−1889.634	INFINITE
100	54.455	34.317	235.233	−20.092	−1896.262	−1853.855	968.355
200	105.922	89.529	148.666	−11.827	−1899.472	−1809.884	472.693
298.15	131.988	137.298	137.298	0.	−1899.536	−1765.817	309.364
300	132.320	138.115	137.300	0.244	−1899.519	−1764.987	307.312
400	144.992	178.096	142.666	14.172	−1898.035	−1720.341	224.653
500	153.841	211.441	153.178	29.131	−1895.852	−1676.159	175.107
600	160.737	240.126	165.334	44.875	−1893.233	−1632.460	142.118
700	166.013	265.318	177.855	61.225	−1890.331	−1589.225	118.589
800	170.038	287.760	190.216	78.035	−1887.259	−1546.418	100.971
900	173.117	307.972	202.195	95.199	−1884.086	−1504.003	87.290
1000	175.502	326.340	213.706	112.634	−1880.865	−1461.944	76.364
1100	177.360	343.157	224.720	130.280	−1877.632	−1420.207	67.440
1200	178.828	358.654	235.244	148.092	−1874.413	−1378.766	60.016
1300	179.991	373.016	245.296	166.035	−1871.225	−1337.591	53.745
1400	180.920	386.390	254.902	184.082	−1868.087	−1296.661	48.379
1500	181.665	398.898	264.090	202.213	−1865.024	−1255.953	43.736
1600	182.263	410.642	272.886	220.410	−1862.060	−1215.445	39.680
1700	182.745	421.707	281.318	238.661	−1859.220	−1175.119	36.107
1785.000	183 .075	430.631	288.217	254.209	--- CRYSTAL <--> LIQUID ---		
1800	183.129	432.163	289.410	256.956	−1856.527	−1134.957	32.936
1900	183.435	442.073	297.187	275.284	−1854.000	−1094.939	30.102
2000	183.678	451.489	304.668	293.640	−1851.656	−1055.050	27.555
2100	183.862	460.455	311.875	312.018	−1849.512	−1015.273	25.254
2200	184.004	469.012	318.825	330.411	−1847.584	−975.592	23.164
2300	184.109	477.193	325.534	348.817	−1845.891	−935.996	21.257

PREVIOUS: CURRENT December 1972

$S°(298.15\ K)$ = [171.488] $J·K^{-1}·mol^{-1}$
T_{fus} = 1785 ± 30 K

$\Delta_f H°(298.15\ K)$ = [−1830.873] $kJ·mol^{-1}$
$\Delta_{fus}H°$ = 104.265 ± 2.1 $kJ·mol^{-1}$

Enthalpy of Formation

$\Delta_f H°(Nb_2O_5, l, 298.15\ K)$ is calculated from that of the crystal by adding $\Delta_{fus}H°$ and the difference in $H°(1785\ K)$–$H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

Orr[1] and Gel'd and Kusenko[2] reported enthalpy measurements at temperatures greater than T_{fus}. The work of Orr[1] indicates a $C_p°$ value of 57.90 $cal·K^{-1}·mol^{-1}$ based on two enthalpy points in the liquid region. The three enthalpy points of Gel'd and Kusenko[2] deviate by +0.06%, −0.86%, and −0.37% from the linear representation of the Orr data. Thus, the constant $C_p°$ value of 57.90 $cal·K^{-1}·mol^{-1}$ is chosen for the liquid phase. A glass transition is also chosen at 1200 K so as to ensure the proper thermodynamic relationship between crystal values and extrapolated liquid value. At temperatures below 1200 K, the heat capacity values of the crystal are used. The entropy at 298.15 K is calculated in a manner analogous to that used in calculating the enthalpy of formation.

Fusion Data

The enthalpy work of Orr[1] and Gel'd and Kusenko[2] provide information as to the heat of fusion. The heat capacity discussion for Nb_2O_5(cr) and Nb_2O_5(l) provide details as to the fitting of the data in the crystal and liquid regions. The heat of fusion is then calculated to be $\Delta_{fus}H°$ = 24.31 ± 0.5 $kcal·mol^{-1}$ at a melting point of 1785 K [$H°(1785\ K)$–$H°(298.15\ K)$ = −60.759 $kcal·mol^{-1}$ for the crystal]. This melting point, although it is consistent with the enthalpy work,[1,2] is 21 K greater than the value reported by Holtzberg *et al.*[3] and is greater than most T_{fus} values cited by Charlesworth[4] and Schneider.[5] Reisman and Holtzberg[6] attributed this high value of 1785 K to an impure sample. The melting point, T_{fus}, is chosen to be 1785 K strictly on the basis of being consistent with the two sets of enthalpy data. More data are necessary to accurately define consistent values for T_{fus}, $\Delta_{fus}H°$, and enthalpy values in the liquid and crystal regions.

References

[1] R. L. Orr, J. Amer. Chem. Soc. 75, 2808 (1953).
[2] P. V. Gel'd and F. G. Kusenko, Izvest. Akad. Nauk SSSR O.T.N. Met. i Top. 1960 (2), 79 (1960); Chem. Abstr. 55, 16117 (1961), data extracted from the following: Ya. I. Gerasimov, A. N. Kustovnikov, and A. S. Shakhov, "Chemical Thermodynamics in Nonferrous Metallurgy," Vol. III, Israel Program for Scientific Translations, Jerusalem, (1965).
[3] F. Holtzberg, A. Reisman, M. Berry, and M. Berkenblit, J. Amer. Chem. Soc. 79, 2039 (1957).
[4] J. H. Charlesworth, AFML-TR-70-137; (October 1970).
[5] S. J. Schneider, U.S. Nat. Bur. Stand. Monograph 68, 31 pp. (1963).
[6] A. Reisman and F. Holtzberg, High Temp. Oxides 2, 217 (1970).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

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							
100							
200							
298.15	131.988	171.488	171.488	0.	−1830.873	−1707.347	299.120
300	132.320	172.306	171.491	0.244	−1830.856	−1706.581	297.142
400	144.992	212.286	176.857	14.172	−1829.371	−1665.354	217.473
500	153.841	245.631	187.368	29.131	−1827.189	−1624.591	169.720
600	160.737	274.316	199.524	44.875	−1824.569	−1584.311	137.927
700	166.013	299.509	212.045	61.225	−1821.668	−1544.495	115.252
800	170.038	321.950	224.406	78.035	−1818.595	−1505.107	98.273
900	173.117	342.162	236.386	95.199	−1815.423	−1466.111	85.091
1000	175.502	360.530	247.896	112.634	−1812.202	−1427.470	74.563
1100	177.360	377.347	258.910	130.280	−1808.969	−1389.153	65.965
1200	178.828	392.845	269.434	148.093	−1805.749	−1351.131	58.813
1200.000	178.828	392.845	269.434	148.093	GLASS <--> LIQUID		
1200.000	242.254	392.845	269.434	148.093	TRANSITION		
1300	242.254	412.236	279.683	172.318	−1796.279	−1313.631	52.782
1400	242.254	430.189	289.800	196.544	−1786.963	−1276.855	47.640
1500	242.254	446.902	299.723	220.769	−1777.804	−1240.739	43.206
1600	242.254	462.537	309.416	244.994	−1768.813	−1205.229	39.347
1700	242.254	477.224	318.859	269.220	−1759.998	−1170.276	35.958
1785.000	242 .254	489.043	326.684	289.811	--- CRYSTAL <--> LIQUID ---		
1800	242.254	491.070	328.045	293.445	−1751.374	−1135.837	32.961
1900	242.254	504.168	336.973	317.670	−1742.951	−1101.871	30.293
2000	242.254	516.594	345.646	341.896	−1734.738	−1068.343	27.902
2100	242.254	528.414	354.071	366.121	−1726.746	−1035.221	25.750
2200	242.254	539.684	362.253	390.347	−1718.985	−1002.472	23.802
2300	242.254	550.452	370.204	414.572	−1711.473	−970.074	22.031
2400	242.254	560.762	377.930	438.797	−1704.227	−937.996	20.415
2500	242.254	570.652	385.443	463.023	−1697.280	−906.214	18.934
2600	242.254	580.153	392.750	487.248	−1690.674	−874.703	17.573
2700	242.254	589.296	399.861	511.473	−1684.489	−843.437	16.317
2800	242.254	598.106	406.785	535.699	−1731.546	−811.424	15.137
2900	242.254	606.607	413.530	559.924	−1723.909	−778.699	14.026
3000	242.254	614.820	420.103	584.149	−1716.320	−746.234	12.993
3100	242.254	622.763	426.513	608.375	−1708.778	−714.021	12.031
3200	242.254	630.455	432.767	632.600	−1701.282	−682.053	11.133
3300	242.254	637.909	438.871	656.826	−1693.829	−650.319	10.294
3400	242.254	645.141	444.832	681.051	−1686.417	−618.807	9.507
3500	242.254	652.163	450.656	705.276	−1679.046	−587.515	8.768
3600	242.254	658.988	456.349	729.502	−1671.713	−556.432	8.074
3700	242.254	665.625	461.915	753.727	−1664.417	−525.554	7.419
3800	242.254	672.086	467.362	777.952	−1657.157	−494.869	6.802
3900	242.254	678.379	472.692	802.178	−1649.932	−464.376	6.220
4000	242.254	684.512	477.911	826.403	−1642.740	−434.070	5.668
4100	242.254	690.494	483.023	850.628	−1635.580	−403.942	5.146
4200	242.254	696.331	488.033	874.854	−1628.452	−373.988	4.651
4300	242.254	702.032	492.944	899.079	−1621.355	−344.203	4.181
4400	242.254	707.601	497.759	923.304	−1614.289	−314.585	3.735
4500	242.254	713.045	502.483	947.530	−1607.253	−285.126	3.310
4600	242.254	718.370	507.119	971.755	−1600.248	−255.824	2.905
4700	242.254	723.580	511.669	995.981	−1593.273	−226.671	2.519
4800	242.254	728.680	516.137	1020.206	−1586.330	−197.668	2.151
4900	242.254	733.675	520.526	1044.431	−1579.418	−168.808	1.800
5000	242.254	738.569	524.838	1068.657	−1572.540	−140.089	1.464

PREVIOUS: CURRENT: December 1972

0 to 1785 K crystal
above 1785 K liquid

Refer to the individual tables for details.

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = p° = 0.1 MPa

	J·K⁻¹·mol⁻¹			kJ·mol⁻¹			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
0	0.	0.	INFINITE	−22.287	−1889.634	−1889.634	INFINITE
100	54.455	34.317	235.233	−20.092	−1896.262	−1853.855	968.355
200	105.922	89.529	148.666	−11.827	−1899.472	−1809.884	472.693
298.15	131.988	137.298	137.298	0.	−1899.536	−1765.817	309.364
300	132.320	138.115	137.300	0.244	−1899.519	−1764.987	307.312
400	144.992	178.096	142.666	14.172	−1898.035	−1720.341	224.653
500	153.841	211.441	153.178	29.131	−1895.852	−1676.159	175.107
600	160.737	240.126	165.334	44.875	−1893.233	−1632.460	142.118
700	166.013	265.318	177.855	61.225	−1890.331	−1589.225	118.589
800	170.038	287.760	190.216	78.035	−1887.259	−1546.418	100.971
900	173.117	307.972	202.195	95.199	−1884.086	−1504.003	87.290
1000	175.502	326.340	213.706	112.634	−1880.865	−1461.944	76.364
1100	177.360	343.157	224.720	130.280	−1877.632	−1420.207	67.440
1200	178.828	358.654	235.244	148.092	−1874.413	−1378.766	60.016
1300	179.991	373.016	245.296	166.035	−1871.225	−1337.591	53.745
1400	180.920	386.390	254.902	184.082	−1868.087	−1296.661	48.379
1500	181.665	398.898	264.090	202.213	−1865.024	−1255.953	43.736
1600	182.263	410.642	272.886	220.410	−1862.060	−1215.445	39.680
1700	182.745	421.707	281.318	238.661	−1859.220	−1175.119	36.107
1785.000	183.075	430.631	288.217	254.209	CRYSTAL <--> LIQUID TRANSITION		
1785.000	242.254	489.043	288.217	358.475			
1800	242.254	491.070	289.899	362.108	−1751.374	−1135.837	32.961
1900	242.254	504.168	300.835	386.334	−1742.951	−1101.871	30.293
2000	242.254	516.594	311.315	410.559	−1734.738	−1068.343	27.902
2100	242.254	528.414	321.374	434.784	−1726.746	−1035.221	25.750
2200	242.254	539.684	331.043	459.010	−1718.985	−1002.472	23.802
2300	242.254	550.452	340.350	483.235	−1711.473	−970.074	22.031
2400	242.254	560.762	349.321	507.461	−1704.227	−937.996	20.415
2500	242.254	570.652	357.977	531.686	−1697.280	−906.214	18.934
2600	242.254	580.153	366.341	555.911	−1690.674	−874.703	17.573
2700	242.254	589.296	374.430	580.137	−1684.489	−843.437	16.317
2800	242.254	598.106	382.262	604.362	−1731.546	−811.424	15.137
2900	242.254	606.607	389.853	628.587	−1723.909	−778.699	14.026
3000	242.254	614.820	397.216	652.813	−1716.320	−746.234	12.993
3100	242.254	622.763	404.364	677.038	−1708.778	−714.021	12.031
3200	242.254	630.455	411.310	701.263	−1701.282	−682.053	11.133
3300	242.254	637.909	418.064	725.489	−1693.829	−650.319	10.294
3400	242.254	645.141	424.637	749.714	−1686.417	−618.807	9.507
3500	242.254	652.163	431.038	773.940	−1679.046	−587.515	8.768
3600	242.254	658.988	437.275	798.165	−1671.713	−556.432	8.074
3700	242.254	665.625	443.358	822.390	−1664.417	−525.554	7.419
3800	242.254	672.086	449.292	846.616	−1657.157	−494.869	6.802
3900	242.254	678.379	455.086	870.841	−1649.932	−464.376	6.220
4000	242.254	684.512	460.745	895.066	−1642.740	−434.070	5.668
4100	242.254	690.494	466.276	919.292	−1635.580	−403.942	5.146
4200	242.254	696.331	471.685	943.517	−1628.452	−373.988	4.651
4300	242.254	702.032	476.975	967.742	−1621.355	−344.203	4.181
4400	242.254	707.601	482.154	991.968	−1614.289	−314.585	3.735
4500	242.254	713.045	487.225	1016.193	−1607.253	−285.126	3.310
4600	242.254	718.370	492.192	1040.418	−1600.248	−255.824	2.905
4700	242.254	723.580	497.060	1064.644	−1593.273	−226.671	2.519
4800	242.254	728.680	501.832	1088.869	−1586.330	−197.668	2.151
4900	242.254	733.675	506.513	1113.095	−1579.418	−168.808	1.800
5000	242.254	738.569	511.105	1137.320	−1572.540	−140.089	1.464

PREVIOUS: CURRENT. December 1972

Continued from page 1676

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