REFERENCE STATE

0	to	1166	K	crystal, alpha
1166	to	1939	K	crystal, beta
1939	to	3630.956	K	liquid
3630.956	to	6000	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

	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	−4.830	0.	0.	0.
100	14.334	8.261	50.955	−4.269	0.	0.	0.
200	22.367	21.227	32.989	−2.352	0.	0.	0.
298.15	25.238	30.759	30.759	0.	0.	0.	0.
300	25.276	30.915	30.760	0.047	0.	0.	0.
400	26.862	38.423	31.772	2.660	0.	0.	0.
500	27.877	44.534	33.733	5.401	0.	0.	0.
600	28.596	49.683	35.973	8.226	0.	0.	0.
700	29.135	54.134	38.257	11.114	0.	0.	0.
800	29.472	58.039	40.490	14.039	0.	0.	0.
900	30.454	61.561	42.639	17.030	0.	0.	0.
1000	32.074	64.848	44.697	20.151	0.	0.	0.
1100	34.334	68.006	46.673	23.466	0.	0.	0.
1166.000	36.175	70.058	47.938	25.791	ALPHA <--> BETA TRANSITION		
1166.000	29.245	73.636	47.938	29.963			
1200	29.459	74.479	48.679	30.961	0.	0.	0.
1300	30.175	76.864	50.756	33.941	0.	0.	0.
1400	31.023	79.131	52.702	37.000	0.	0.	0.
1500	32.003	81.304	54.537	40.150	0.	0.	0.
1600	33.115	83.404	56.276	43.405	0.	0.	0.
1700	34.359	85.448	57.932	46.778	0.	0.	0.
1800	35.736	87.451	59.517	50.281	0.	0.	0.
1900	37.244	89.422	61.039	53.929	0.	0.	0.
1939.000	37.868	90.186	61.617	55.394	BETA <--> LIQUID TRANSITION		
1939.000	47.237	97.481	61.617	69.540			
2000	47.237	98.944	62.734	72.421	0.	0.	0.
2100	47.237	101.249	64.513	77.145	0.	0.	0.
2200	47.237	103.446	66.233	81.869	0.	0.	0.
2300	47.237	105.546	67.897	86.592	0.	0.	0.
2400	47.237	107.557	69.508	91.316	0.	0.	0.
2500	47.237	109.485	71.069	96.040	0.	0.	0.
2600	47.237	111.338	72.582	100.764	0.	0.	0.
2700	47.237	113.120	74.051	105.487	0.	0.	0.
2800	47.237	114.838	75.477	110.211	0.	0.	0.
2900	47.237	116.496	76.863	114.935	0.	0.	0.
3000	47.237	118.097	78.211	119.659	0.	0.	0.
3100	47.237	119.646	79.523	124.382	0.	0.	0.
3200	47.237	121.146	80.800	129.106	0.	0.	0.
3300	47.237	122.600	82.045	133.830	0.	0.	0.
3400	47.237	124.010	83.259	138.554	0.	0.	0.
3500	47.237	125.379	84.443	143.277	0.	0.	0.
3600	47.237	126.710	85.598	148.001	0.	0.	0.
3630.956	47.237	127.114	85.951	149.463	LIQUID <--> IDEAL GAS FUGACITY = 1 bar		
3630.956	34.219	240.028	85.951	559.447			
3700	34.613	240.676	88.832	561.823	0.	0.	0.
3800	35.173	241.607	92.840	565.313	0.	0.	0.
3900	35.721	242.527	96.667	568.857	0.	0.	0.
4000	36.254	243.439	100.324	572.456	0.	0.	0.
4100	36.772	244.340	103.826	576.108	0.	0.	0.
4200	37.273	245.232	107.182	579.810	0.	0.	0.
4300	37.757	246.115	110.403	583.562	0.	0.	0.
4400	38.223	246.988	113.497	587.361	0.	0.	0.
4500	38.670	247.852	116.473	591.206	0.	0.	0.
4600	39.097	248.707	119.339	595.094	0.	0.	0.
4700	39.505	249.552	122.100	599.025	0.	0.	0.
4800	39.892	250.388	124.764	602.995	0.	0.	0.
4900	40.259	251.214	127.336	607.002	0.	0.	0.
5000	40.606	252.031	129.822	611.046	0.	0.	0.
5200	41.240	253.637	134.554	619.232	0.	0.	0.
5400	41.796	255.204	138.993	627.537	0.	0.	0.
5600	42.277	256.733	143.171	635.945	0.	0.	0.
5800	42.686	258.224	147.113	644.443	0.	0.	0.
6000	43.029	259.677	150.841	653.015	0.	0.	0.

PREVIOUS: June 1979 (1 atm) CURRENT: June 1979 (1 bar)

$S°(298.15\ K) = 30.759 \pm 0.2\ J \cdot K \cdot mol^{-1}$
$T_{tr} = 1166 \pm 10\ K\ (\alpha–\beta)$

$\Delta_f H°(0\ K) = 0\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = 0\ kJ \cdot mol^{-1}$
$\Delta_{tr} H° = 0.997 \pm 0.03\ kJ \cdot mol^{-1}$

Enthalpy of Formation

Zero by definition

Heat Capacity and Entropy

The adopted thermal functions for α–Ti(cr) are derived from the studies of Collings and Ho,[1] Clusius and Franzosini,[2] Stalinski and Bieganski,[3] Scott,[4] Backhurst[5] and Cezairliyan and Miiller.[6] The mathematical and graphical treatment of these four studies yields a continuous and smooth heat capacity curve.

There are ten studies[1,7–15] on the heat capacity of titanium in the range 1–5 K. Wolcott[9] and Aven *et al*.[8] reported the experimental data. In the other studies, an equation (with two constants) was given to describe the entire set of experimental data. The constants given by Collings and Ho[1] agree with the experimental data of Wolcott[9] and of Aven *et al*.[8] The maximum difference in the calculated values for $S°(5\ K)$ is $0.00071\ cal \cdot K^{-1} \cdot mol^{-1}$, with the adopted value being $S°(5\ K) = 0.0043\ cal \cdot K^{-1} \cdot mol^{-1}$. Similarly for $C_p°(5\ K)$ the maximum difference is $0.00211\ cal \cdot K^{-1} \cdot mol^{-1}$, with the adopted value being $C_p°\ (5\ K) = 0.0049\ cal \cdot K^{-1} \cdot mol^{-1}$.

In the region above 5 K and below 360 K, there are seven heat capacity studies.[2,3,8,9–18] The adopted values were based on the work of Clusius and Franzosini[2] and Stalinski and Bieganski.[3] The maximum deviation of all studies from the adopted is 2.5% over this temperature range.

Above 300 K, there are eleven heat capacity studies[4–6,18–25] and seven enthalpy studies.[26–32] The heat capacity studies all have a similar temperature dependence in comparison with the adopted values. However, the studies of Holland,[19] Affortit,[23] Arutyunov,[24] and Rumyantsev *et al*.[25] lie roughly 9–33% higher than the adopted values. There is much scatter in all studies within 50 K of the α–β transition temperature. The adopted values were based on Scott,[4] Backhurst[5], and Cezairliyan and Miller.[6] The enthalpy studies show a large scatter within each study as well as a general lack of agreement between the studies.

Transition Data

Refer to the β–crystal table for details.

Sublimation Data

There are no sublimation studies involving α–Ti(cr). The enthalpy of sublimation is calculated as the difference between the enthalpy of formation of the monatomic gas and the enthalpy of formation of α–Ti(cr).

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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	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−4.830	0.	0.	0.
100	14.334	8.261	50.955	−4.269	0.	0.	0.
200	22.367	21.227	32.989	−2.352	0.	0.	0.
250	24.074	26.414	31.169	−1.189	0.	0.	0.
298.15	25.238	30.759	30.759	0.	0.	0.	0.
300	25.276	30.915	30.760	0.047	0.	0.	0.
350	26.169	34.882	31.071	1.334	0.	0.	0.
400	26.862	38.423	31.772	2.660	0.	0.	0.
450	27.418	41.620	32.692	4.018	0.	0.	0.
500	27.877	44.534	33.733	5.401	0.	0.	0.
600	28.596	49.683	35.973	8.226	0.	0.	0.
700	29.135	54.134	38.257	11.114	0.	0.	0.
800	29.472	58.039	40.490	14.039	0.	0.	0.
900	30.454	61.561	42.639	17.030	0.	0.	0.
1000	32.074	64.848	44.697	20.151	0.	0.	0.
1100	34.334	68.006	46.673	23.466	0.	0.	0.
1166.000	36.175	70.058	47.938	25.791	---- ALPHA <--> BETA ----		
1200	37.233	71.113	48.580	27.039	−3.922	0.118	−0.005
1300	40.771	74.228	50.433	30.934	−3.007	0.420	−0.017
1400	44.948	77.399	52.245	35.214	−1.786	0.640	−0.024
1500	49.764	80.660	54.030	39.945	−0.205	0.760	−0.026
1600	55.220	84.043	55 800	45 189	1.784	0.762	−0.025
1700	61.314	87.570	57.564	51.010	4.232	0.625	−0.019

PREVIOUS: September 1966 CURRENT: June 1979

$S°(298.15\ K)$ = [38.122] $J·K^{-1}·mol^{-1}$
T_{trs} = 1166 ± 10 K (α–β)
T_{fus} = 1939 ± 10 K (β–l)

$\Delta_f H°(298.15\ K)$ = [6.860] $kJ·mol^{-1}$
$\Delta_{trs}H°$ = 4.172 ± 0.13 $kJ·mol^{-1}$
$\Delta_{fus}H°$ = 14.146 ± 5.0 $kJ·mol^{-1}$

Enthalpy of Formation

The enthalpy of formation is calculated from that of the α–crystal by addition of $\Delta_{trs}H°$ and the difference in enthalpy, $H°(1166\ K)-H°(298.15\ K)$, between the α–crystal and the β–crystal.

Heat Capacity and Entropy

For the β–crystal there are ten heat capacity studies and six enthalpy studies. The discussion on heat capacity and enthalpy on the α–Ti(cr) table also applies to the β–Ti(cr).

The entropy at 298.15 K is calculated in a manner similar to that for the enthalpy of formation.

Phase Data

Titanium, at ambient pressures, exists in two crystal modifications. The low temperature form, α–Ti, is hexagonal close packed, an hcp (A3) structure isotypic with Mg. The high temperature form, β–Ti, is body centered cubic, a bcc (A2) structure isotypic with W.

Transition Data

The following table indicates the values of transition temperatures and enthalpies of transition reported by various investigators. The value of T_{trs} adoped is 1166 ± 10 K, and the value of $\Delta_{trs}H°$ is selected as 0.997 ± 0.03 $kcal·mol^{-1}$, based on the work of Cezairliyan and Miller.[1]

Source	T_{trs}/K	$\Delta_{trs}H°$, $kcal·mol^{-1}$	Purity, %	Method
Fast[2]	1158 ± 10		Iodide	electrical resistance
Greiner and Ellis[3]	1158 ± 2		99.9	electrical resitance
McQuillan[4]	1155.7 ± 1	0.67	99.93	hydrogen solubility
Worner[5]	1158 ± 2		99.93	thermoelectric power
Duwez[6]	1155 ± 4		Iodide	cooling curve
Kothen[7]	1154	0.943	99.96	drop calorimetry
Edwards *et al.*[8]	1157 ± 3.5		99.88	cooling curve
Schofield[9]	1158	0.814	—	rate of heating
Scott[10]	1156 ± 2	0.978 ± 0.025	Iodide	adiabatic calorimetry
Backhurst[11]	1165–1179	0.88	Commercial	adiabatic calorimetry
Golutvin[12]	1155	0.82 ± .020	Iodide	drop calorimetry
Kohlhaas *et al.*[13]	1167	0.992	99.8	adiabatic calorimetry
Gel'd and Putintsev[14]		0.998		
Martynyuk and Tsapkov[15]		1.028	99.74	pulsed heating
Harmelin and Lehr[16]		1.007		DTA
Etchessahar and Debuigne[17]	1154			dilatometric
Cezairliyan and Miller[1]	1166	0.997	99.9+	electrical resistance

Fusion Data

Refer to the liquid table for details.

Sublimation Data

There are three sublimation studies involving β–Ti(cr). They are summarized on the ideal gas table. The enthalpy of sublimation for β–Ti(cr) is calculated as the difference in the enthalpies of formation at 298.15 K of Ti(g) and β–Ti(cr).

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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	23.995	38.122	38.122	0.	6.860	4.665	−0.817
300	24.006	38.271	38.123	0.044	6.858	4.652	−0.810
350	24.309	41.994	38.416	1.252	6.779	4.290	−0.640
400	24.611	45.260	39.071	2.475	6.675	3.941	−0.515
450	24.914	48.176	39.924	3.713	6.556	3.606	−0.419
500	25.216	50.816	40.883	4.967	6.427	3.285	−0.343
600	25.821	55.467	42.937	7.519	6.153	2.682	−0.234
700	26.426	59.493	45.020	10.131	5.877	2.126	−0.159
800	27.031	63.061	47.057	12.804	5.625	1.607	−0.105
900	27.636	66.280	49.017	15.537	5.368	1.120	−0.065
1000	28.241	69.223	50.892	18.331	5.040	0.665	−0.035
1100	28.846	71.943	52.684	21.185	4.580	0.248	−0.012
1166.000	29.245	73.636	53.822	23.102	---- ALPHA <--> BETA ----		
1200	29.459	74.479	54.396	24.100	0.	0.	0.
1300	30.175	76.864	56.033	27.081	0.	0.	0.
1400	31.023	79.131	57.603	30.140	0.	0.	0.
1500	32.003	81.304	59.111	33.290	0.	0.	0.
1600	33.115	83.404	60.564	36.544	0.	0.	0.
1700	34.359	85.448	61.968	39.917	0.	0.	0.
1800	35.736	87.451	63.328	43.421	0.	0.	0.
1900	37.244	89.422	64.650	47.069	0.	0.	0.
1939.000	37.868	90.186	65.155	48.533	---- BETA <--> LIQUID ----		
2000	38.885	91.374	65.937	50.874	−14.687	0.454	−0.012
2100	40.657	93.314	67.195	54.850	−15.435	1.230	−0.031
2200	42.562	95.248	68.426	59.010	−15.998	2.037	−0.048
2300	44.599	97.185	69.634	63.367	−16.365	2.866	−0.065
2400	46.768	99.128	70.822	67.934	−16.522	3.706	−0.081
2500	49.069	101.084	71.994	72.725	−16.455	4.549	−0.095

PREVIOUS: September 1966 CURRENT: June 1979

$S°(298.15\ K)$ = [39.181] $J·K^{-1}·mol^{-1}$
T_{fus} = 1936 ± 10 K

$\Delta_f H°(298.15\ K)$ = [13.652] $kJ·mol^{-1}$
$\Delta_{fus}H°$ = 14.146 ± 5.0 $kJ·mol^{-1}$

Enthalpy of Formation

The enthalpy of formation is calculated from that of the β–crystal by addition of $\Delta_{fus}H°$ and the difference in enthalpy, $H°(1936\ K)–H°(198.15\ K)$, between the β–crystal and the liquid.

Heat Capacity and Entropy

There are two enthalpy studies[1,2] covering the liquid region of titanium. The work of Treverton and Margrave[1] was adopted. A glass transition is assumed at 1300 K below which extrapolated β–Ti heat capacity values are used. The entropy is calculated in a manner similar to that used for the enthalpy of formation.

Fusion Data

The investigators reporting melting temperatures and heats of melting are listed below. The value of T_{fus} adopted is 1939 ± 10 K, and the value of $\Delta_{fus}H°$ is selected as 3.381 ± 0.03 kcal·mol^{-1}, based on the work of Berezin *et al.*[2,13]

Source	T_{fus}/K	$\Delta_{fus}H°$ kcal·mol^{-1}
Burgess and Waltenburg[3]	2068	
Fast[4]	1993	
Adenstedt *et al.*[5]	1973	
Hansen *et al.*[6]	1993	
Maykuth *et al.*[7]	1953	
Schofield and Bacon[8]	1933	
Oriani and Jones[9]	1945	
Deardorff and Hayes[10]	1941	
Westrum and Feick[11]	1933	
Elyutin *et al.*[12]	1941	4.1 ± 0.1
Treverton and Margrave[1]	1943	3.161 ± 0.12
Berezin *et al.*[13]	1939	3.381 ± 0.115

Vaporization Data

The two vaporization studies are summarized on the ideal gas table. The boiling point is calculated as that temperature for which $\Delta G° = 0$ for Ti(l) = Ti(g). $\Delta_{vap}H°$ is the corresponding enthalpy change. T_{vap} is the temperature at which fugacity is one bar. The normal boiling point (p=1 bar) would be a slightly lower temperature.

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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	27.638	39.181	39.181	0.	13.652	11.141	−1.952
300	27.639	39.352	39.181	0.051	13.657	11.126	−1.937
350	27.667	43.614	39.518	1.434	13.752	10.696	−1.596
400	27.694	47.310	40.266	2.818	13.810	10.255	−1.339
450	27.722	50.574	41.234	4.203	13.838	9.809	−1.139
500	27.750	53.496	42.316	5.590	13.842	9.360	−0.978
600	27.805	58.560	44.614	8.368	13.794	8 468	−0.737
700	27.860	62.851	46.921	11.151	13.689	7.587	−0.566
800	27.916	66.573	49.150	13.939	13.552	6.725	−0.439
900	28.104	69.871	51.272	16.739	13.361	5.882	−0.341
1000	28.423	72.847	53.283	19.564	13.065	5.066	−0.265
1100	28.875	75.576	55.188	22.428	12.614	4.286	−0.204
1200	29.459	78.113	56.993	25.343	8.035	3.674	−0.160
1300	30.175	80.498	58.711	28.324	8.035	3.311	−0.133
1400	31.023	82.765	60.348	31.383	8.035	2.948	−0.110
1460.000	31.595	84.078	61.297	33.261	GLASS <--> LIQUID		
1460.000	47.237	84.078	61.297	33.261	TRANSITION		
1500	47.237	85.355	61.921	35.150	8.652	2.576	−0.090
1600	47.237	88.404	63.482	39.874	10.121	2.122	−0.069
1700	47.237	91.267	65.033	44.598	11.473	1.580	−0.049
1800	47.237	93.967	66.566	49.321	12.693	0.962	−0.028
1900	47.237	96.521	68.076	54.045	13.768	0.281	−0.008
1939.000	47.237	97.481	68.658	55.887	BETA <--> LIQUID		
2000	47.237	98.944	69.560	58.769	0.	0.	0.
2100	47.237	101.249	71.014	63.493	0.	0.	0.
2200	47.237	103.446	72.439	68.216	0.	0.	0.
2300	47.237	105.546	73.833	72.940	0.	0.	0.
2400	47.237	107.557	75.197	77.664	0.	0.	0.
2500	47.237	109.485	76.530	82.388	0.	0.	0.
2600	47.237	111.338	77.833	87.111	0.	0.	0.
2700	47.237	113 120	79.107	91 835	0.	0.	0.
2800	47.237	114.838	80.353	96.559	0.	0.	0.
2900	47.237	116.496	81.571	101.283	0.	0.	0.
3000	47.237	118.097	82.762	106.006	0.	0.	0.
3100	47.237	119.646	83.927	110.730	0.	0.	0.
3200	47.237	121.146	85.067	115.454	0.	0.	0.
3300	47.237	122.600	86.182	120.178	0.	0.	0.
3400	47.237	124.010	87.274	124.901	0.	0.	0.
3500	47.237	125.379	88.343	129.625	0.	0.	0.
3600	47.237	126.710	89.391	134.349	0.	0.	0.
3630.956	47.237	127.114	89.711	135.811	FUGACITY = 1 bar		
3700	47.237	128.004	90.417	139.072	−409.098	7.788	−0.110
3800	47.237	129.264	91.423	143.796	−407.864	19.039	−0.262
3900	47.237	130.491	92.409	148.520	−406.685	30.258	−0.405
4000	47.237	131.687	93.376	153.244	−405.560	41.447	−0.541
4100	47.237	132.853	94.324	157.967	−404.488	52.609	−0.670
4200	47.237	133.991	95.255	162.691	−403.467	63.745	−0.793
4300	47.237	135.103	96.169	167.415	−402.495	74.858	−0.909
4400	47.237	136.189	97.066	172.139	−401.570	85.948	−1.020
4500	47.237	137.250	97.948	176.862	−400.691	97.018	−1.126

PREVIOUS: September 1966 CURRENT: June 1979

0	to	1166	K crystal, alpha
1166	to	1936	K crystal, beta
above		1936	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	−4.830	0.	0.	0.
100	14.334	8.261	50.955	−4.269	0.	0.	0.
200	22.367	21.227	32.989	−2.352	0.	0.	0.
250	24.074	26.414	31.169	−1.189	0.	0.	0.
298.15	25.238	30.759	30.759	0.	0.	0.	0.
300	25.276	30.915	30.760	0.047	0.	0.	0.
350	26.169	34.882	31.071	1.334	0.	0.	0.
400	26.862	38.423	31.772	2.660	0.	0.	0.
450	27.418	41.620	32.692	4.018	0.	0.	0.
500	27.877	44.534	33.733	5.401	0.	0.	0.
600	28.596	49.683	35.973	8.226	0.	0.	0.
700	29.135	54.134	38.257	11.114	0.	0.	0.
800	29.472	58.039	40.490	14.039	0.	0.	0.
900	30.454	61.561	42.639	17.030	0.	0.	0.
1000	32.074	64.848	44.697	20.151	0.	0.	0.
1100	34.334	68.006	46.673	23.466	0.	0.	0.
1166.000	36.175	70.058	47.938	25.791	ALPHA <--> BETA TRANSITION		
1166.000	29.245	73.636	47.938	29.963			
1200	29.459	74.479	48.679	30.961	0.	0.	0.
1300	30.175	76.864	50.756	33.941	0.	0.	0.
1400	31.023	79.131	52.702	37.000	0.	0.	0.
1500	32.003	81.304	54.537	40.150	0.	0.	0.
1600	33.115	83.404	56.276	43.405	0.	0.	0.
1700	34.359	85.448	57.932	46.778	0.	0.	0.
1800	35.736	87.451	59.517	50.281	0.	0.	0.
1900	37.244	89.422	61.039	53.929	0.	0.	0.
1939.000	37.868	90.186	61.617	55.394	BETA <--> LIQUID TRANSITION		
1939.000	47.237	97.481	61.617	69.540			
2000	47.237	98.944	62.734	72.421	0.	0.	0.
2100	47.237	101.249	64.513	77.145	0.	0.	0.
2200	47.237	103.446	66.233	81.869	0.	0.	0.
2300	47.237	105.546	67.897	86.592	0.	0.	0.
2400	47.237	107.557	69.508	91.316	0.	0.	0.
2500	47.237	109.485	71.069	96.040	0.	0.	0.
2600	47.237	111.338	72.582	100.764	0.	0.	0.
2700	47.237	113.120	74.051	105.487	0.	0.	0.
2800	47.237	114.838	75.477	110.211	0.	0.	0.
2900	47.237	116.496	76.863	114.935	0.	0.	0.
3000	47.237	118.097	78.211	119.659	0.	0.	0.
3100	47.237	119.646	79.523	124.382	0.	0.	0.
3200	47.237	121.146	80.800	129.106	0.	0.	0.
3300	47.237	122.600	82.045	133.830	0.	0.	0.
3400	47.237	124.010	83.259	138.554	0.	0.	0.
3500	47.237	125.379	84.443	143.277	0.	0.	0.
3600	47.237	126.710	85.598	148.001	0.	0.	0.
3630.956	47.237	127.114	85.951	149.463	FUGACITY = 1 bar		
3700	47.237	128.004	86.727	152.725	−409.098	7.788	−0.110
3800	47.237	129.264	87.830	157.449	−407.864	19.039	−0.262
3900	47.237	130.491	88.908	162.172	−406.685	30.258	−0.405
4000	47.237	131.687	89.963	166.896	−405.560	41.447	−0.541
4100	47.237	132.853	90.995	171.620	−404.488	52.609	−0.670
4200	47.237	133.991	92.005	176.343	−403.467	63.745	−0.793
4300	47.237	135.103	92.994	181.067	−402.495	74.857	−0.909
4400	47.237	136.189	93.964	185.791	−401.570	85.948	−1.020
4500	47.237	137.250	94.914	190.515	−400.691	97.018	−1.126

PREVIOUS: CURRENT: June 1979

IP(Ti, g) = 55010 ± 100 cm^{-1}
$S°(298.15K)$ = 180.297 ± 0.03 $J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K)$ = 470.92 ± 16.7 $kJ·mol^{-1}$
$\Delta_f H°(298.15K)$ = 473.63 ± 16.7 $kJ·mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^3F_2$	0.00	5
$^3F_3$	170.132	7
$^3F_4$	386.874	9
.	.	.
.	.	.
.	.	.
.	.	.
.	.	.
$^1P_1$	53663.32	3
IP	55010	

Enthalpy of Formation

The value adopted for the enthalpy of formation of Ti(g) is that recommended by CODATA.[1] It is obtained from a 2nd and 3rd law evaluation of the vapor pressure data of Wu and Wahlbeck,[2] Berstein and Kaufman,[3] Koch *et al.*,[4] Strassmair and Stark,[5] and Edwards *et al.*[6]

Source	Reaction	T/K	Data Points	$\Delta_f H°$(298.15K), kcal·mol^{-1} 2nd law	3rd law	Drift cal·K^{-1}·mol^{-1}	$\Delta_f H°$(298.15K) kcal·mol^{-1}
Edwards *et al.*[6]	a	1587–1764	8	112.0 ± 1.1	111.5 ± 0.2	−0.3 ± 0.6	113.1
Strassmair and Stark[5]	a	1554–1772	8	111.4 ± 3.5	109.8 ± 0.8	−1.0 ± 2.1	111.4
Wu and Wahlbeck[2]	a	1830–1923	16	112.2 ± 9.3	111.6 ± 1.0	−0.3 ± 4.9	113.2
Koch *et al.*[4]	b	1955–2379	21*	110.9 ± 2.4	109.2 ± 1.3	−0.8 ± 1.1	112.46
Bernstein and Kaufman[3]	b	2000–3000	Smooth	110.6	109.0	−0.6	112.3

*Two points deleted due to a statistical test Reaction. a) Ti(β) = Ti(g) b) Ti(l) = Ti(g)

Heat Capacity and Entropy

The electronic energy levels are given in the recent compilation by Corliss and Sugar.[7] Although we have listed only the ground state, first two excited states, the highest observed excited state, and the ionization potential for Ti(g), all levels listed by Corliss and Sugar,[7] as well as estimated levels, are used in the calculation. The observed levels are too numerous to list completely. In our calculations, the missing levels for $n = 4$, $n = 5$, and $n = 6$ have been arbitrarily added near the ionization limit. Our calculations indicate that for Ti(g) the thermochemical functions are independent of the estimated missing levels (for n = 4,5,6) and the cut–off procedure up to 3000 K. The Gibbs energy function is essentially unaffected (<0.002 cal·K^{-1}·mol^{-1}) at 6000 K. The reported uncertainty in $S°$(298.15K) is due to uncertainties in the relative atomic mass and the fundamental constants. Extension of these calculations above 6000 K may require consideration of the higher excited states ($n > 6$), more precise estimation of missing states (all n), and utilization of proper fill and cut–off procedures.[8] In fact, the inclusion of some higher states (n = 4,5,6) and consideration of various cut–off procedures leads to calculational differences in the Gibbs energy function of rougly 0.1 cal·K^{-1}·mol^{-1}) or greater at temperatures near 10000 K.

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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	0.	0.	INFINITE	−7.539	470.920	470.920	INFINITE
100	26.974	151.246	203.383	−5.214	472.684	458.386	−239.436
200	26.487	170.126	182.593	−2.493	473.488	443.708	−115.885
250	25.355	175.913	180.704	−1.198	473.620	436.245	−91.148
298.15	24.430	180.297	180.297	0.	473.629	429.044	−75.167
300	24.399	180.448	180.297	0.045	473.627	428.768	−74.655
350	23.661	184.151	180.591	1.246	473.541	421.297	−62.875
400	23.104	187.272	181.236	2.414	473.383	413.843	−54.042
450	22.683	189.968	182.060	3.558	473.169	406.413	−47.175
500	22.360	192.340	182.972	4.684	472.912	399.009	−41.684
600	21.913	196.374	184.881	6.896	472.299	384.284	−33.455
700	21.632	199.729	186.769	9.072	471.587	369.670	−27.585
800	21.454	202.605	188.573	11.226	470.816	355.163	−23.190
900	21.353	205.126	190.275	13.366	469.965	340.756	−19.777
1000	21.323	207.373	191.875	15.499	468.977	326.451	−17.052
1100	21.362	209.407	193.377	17.633	467.795	312.254	−14.828
1200	21.474	211.270	194.792	19.774	462.442	298.293	−12.984
1300	21.657	212.996	196.127	21.930	461.617	284.647	−11.437
1400	21.910	214.609	197.390	24.107	460.736	271.066	−10.114
1500	22.228	216.132	198.589	26.314	459.793	257.551	−8.969
1600	22.604	217.578	199.731	28.555	458.779	244.101	−7.969
1700	23.029	218.961	200.822	30.836	457.688	230.717	−7.089
1800	23.497	220.290	201.867	33.162	456.510	217.399	−6.309
1900	23.999	221.574	202.870	35.537	455.237	204.149	−5.612
2000	24.529	222.818	203.837	37.963	439.171	191.423	−4.999
2100	25.080	224.028	204.769	40.443	436.927	179.091	−4.455
2200	25.648	225.208	205.672	42.979	434.740	166.864	−3.962
2300	26.228	226.361	206.546	45.573	432.610	154.736	−3.514
2400	26.819	227.489	207.396	48.225	430.538	142.699	−3.106
2500	27.416	228.596	208.221	50.937	428.526	130.748	−2.732
2600	28.019	229.683	209.026	53.709	426.574	118.875	−2.388
2700	28.626	230.752	209.811	56.541	424.683	107.077	−2.072
2800	29.235	231.804	210.578	59.434	422.852	95.347	−1.779
2900	29.846	232.841	211.328	62.388	421.082	83.682	−1.507
3000	30.456	233.863	212.062	65.403	419.374	72.077	−1.255
3100	31.065	234.871	212.781	68.479	417.726	60.528	−1.020
3200	31.671	235.867	213.487	71.616	416.139	49.031	−0.800
3300	32.273	236.851	214.180	74.813	414.612	37.582	−0.595
3400	32.870	237.823	214.861	78.071	413.146	26.179	−0.402
3500	33.460	238.785	215.531	81.387	411.739	14.818	−0.221
3600	34.042	239.736	216.190	84.762	410.390	3.497	−0.051
3630.956	34.219	240.028	216.392	85.819	----- FUGACITY = 1 bar -----		
3700	34.613	240.676	216.840	88.195	0.	0.	0.
3800	35.173	241.607	217.479	91.685	0.	0.	0.
3900	35.721	242.527	218.110	95.229	0.	0.	0.
4000	36.254	243.439	218.731	98.828	0.	0.	0.
4100	36.772	244.340	219.345	102.480	0.	0.	0.
4200	37.273	245.232	219.951	106.182	0.	0.	0.
4300	37.757	246.115	220.549	109.934	0.	0.	0.
4400	38.223	246.988	221.140	113.733	0.	0.	0.
4500	38.670	247.852	221.724	117.578	0.	0	0.
4600	39.097	248.707	222.301	121.466	0.	0.	0.
4700	39.505	249.552	222.872	125.397	0.	0.	0.
4800	39.892	250.388	223.437	129.367	0.	0.	0.
4900	40.259	251.214	223.995	133.374	0.	0.	0.
5000	40.606	252.031	224.548	137.418	0.	0.	0.
5100	40.933	252.839	225.095	141.495	0.	0.	0.
5200	41.240	253.637	225.636	145.604	0.	0.	0.
5300	41.528	254.425	226.172	149.742	0.	0.	0.
5400	41.796	255.204	226.702	153.909	0.	0.	0.
5500	42.046	255.973	227.227	158.101	0.	0.	0.
5600	42.277	256.733	227.747	162.317	0.	0.	0.
5700	42.490	257.483	228.263	166.556	0.	0.	0.
5800	42.686	258.224	228.773	170.815	0.	0.	0.
5900	42.866	258.955	229.278	175.092	0.	0.	0.
6000	43.029	259.677	229.779	179.387	0.	0.	0.

PREVIOUS: June 1979 (1 atm) CURRENT: June 1979 (1 bar)

$IP(Ti^+, g) = 109500 \pm 1000\ cm^{-1}$
$S°(298.15K) = 183.594 \pm 0.04\ J \cdot K^{-1} mol^{-1}$

$\Delta_f H°(0\ K) = 1128.985 \pm 6.3\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15K) = [1138.252]\ kJ \cdot mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^4F_{3/2}$	0.00	4
$^4F_{5/2}$	93.94	6
$^4F_{7/2}$	225.47	8
$^4F_{9/2}$	393.22	10
.	.	.
.	.	.
.	.	.
$^2F_{7/2}$	70893.00	8
IP	109500	

Enthalpy of Formation

$\Delta_f H°(Ti^+, g, 0\ K)$ is calaculated from $\Delta_f H°(Ti, g, 0\ K)$[1] using the spectroscopic value of $IP(Ti) = 55010 \pm 100\ cm^{-1}$ ($658.07 \pm 0.4\ kJ \cdot mol^{-1}$) from Corliss and Sugar.[2] The ionization limit is converted from cm^{-1} to $kJ \cdot mol^{-1}$ using the factor, $1\ cm^{-1} = 0.01196266\ kJ\ cm^{-1}$, which is derived from the 1973 CODATA fundamental constants.[3] Rosenstock *et al.*[4] and Levine amd Lias[5] have summarized additional ionization and appearance potential data.

$\Delta_f H°(Ti^+, g, 298.15K)$ is calculated from $\Delta_f H°(Ti, g, 0\ K)$ by using IP(Ti) with JANAF[1] enthalpies, $H°(0\ K) - H°(298.15K)$, for Ti(g), $Ti^+(g)$, and $e^-(g)$. $\Delta_f H°(Ti \rightarrow Ti^+ + e^-, 298.15K)$ 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 $-6.197\ kJ \cdot mol^{-1}$ if it is to be used in this ion convention that excludes the enthalpy of the electron.

Heat Capacity and Entropy

The electronic energy levels are given in the recent compilation by Corliss and Sugar.[2] Although we have listed only the ground state, the first three excited states, the highest observed excited state, and the ionization potential for $Ti^+(g)$, all levels listed by Corliss and Sugar,[2] as well as estimated levels, are used in the calculation. The observed levels are too numerous to list completely. In our calculations the missing levels for $n = 4,5$ have been arbitrarily added near the ionization limit. The calculations indicate that for $Ti^+(g)$, the thermochemical functions are independent of the estimated missing levels for $n = 4,5$, the cut–off procedure, and the inclusion of $n = 6$ levels up to 6000 K. The Gibbs energy function is essentially unaffected (by less than 0.2%) up to 20000 K. The reported uncertainty in $S°(298.15K)$ is due to uncertainties in the relative atomic mass and the fundamental constants. Extension of these calculations above 6000 K may require consideration of the higher excited states (n>6), and use of proper fill and cut–off procedures.[6]

References

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

T/K	$C_p°$ ($J \cdot K^{-1} mol^{-1}$)	$S°$ ($J \cdot K^{-1} mol^{-1}$)	$-[G°-H°(T_r)]/T$ ($J \cdot K^{-1} mol^{-1}$)	$H°-H°(T_r)$ ($kJ \cdot mol^{-1}$)	$\Delta_f H°$ ($kJ \cdot mol^{-1}$)	$\Delta_f G°$ ($kJ \cdot mol^{-1}$)	log K_f
0	0.	0.	INFINITE	−7.899	1128.985		
100	28.375	153.817	207.355	−5.354			
200	26.772	173.059	185.998	−2.588			
250	26.305	178.974	184.025	−1.263			
298.15	26.181	183.594	183.594	0.	1138.252	1086.429	−190.338
300	26.180	183.756	183.595	0.048	1138.292	1086.108	−189.108
350	26.166	187.790	183.913	1.357	1139.353	1077.326	−160.782
400	26.128	191.282	184.621	2.665	1140.373	1068.395	−139.518
450	26.021	194.354	185.535	3.969	1141.359	1059.338	−122.965
500	25.843	197.087	186.556	5.265	1142.312	1050.173	−109.711
600	25.356	201.758	188.714	7.826	1144.126	1031.573	−89.806
700	24.817	205.626	190.862	10.335	1145.826	1012.678	−75.567
800	24.320	208.907	192.917	12.791	1147.436	993.546	−64.872
900	23.903	211.746	194.855	15.202	1148.934	974.218	−56.542
1000	23.572	214.247	196.672	17.575	1150.264	954.732	−49.870
1100	23.322	216.481	198.373	19.919	1151.372	935.123	−44.405
1200	23.145	218.502	199.968	22.242	1148.279	915.543	−39.853
1300	23.030	220.350	201.465	24.550	1149.685	896.091	−36.005
1400	22.970	222.054	202.876	26.850	1151.004	876.534	−32.704
1500	22.959	223.638	204.208	29.146	1152.229	856.886	−29.839
1600	22.992	225.121	205.469	31.443	1153.350	837.159	−27.330
1700	23.065	226.517	206.667	33.745	1154.358	817.365	−25.115
1800	23.173	227.838	207.806	36.057	1155.245	797.516	−23.143
1900	23.313	229.095	208.894	38.381	1156.000	777.621	−21.378
2000	23.480	230.295	209.934	40.721	1141.926	758.144	−19.801
2100	23.670	231.445	210.931	43.078	1141.638	738.962	−18.381
2200	23.879	232.551	211.889	45.455	1141.370	719.793	−17.090
2300	24.104	233.617	212.811	47.854	1141.124	700.636	−15.912
2400	24.340	234.648	213.699	50.276	1140.901	681.489	−14.832
2500	24.583	235.646	214.557	52.722	1140.702	662.351	−13.839
2600	24.832	236.615	215.387	55.193	1140.527	643.221	−12.922
2700	25.082	237.557	216.191	57.689	1140.378	624.096	−12.074
2800	25.331	238.474	216.970	60.209	1140.254	604.977	−11.286
2900	25.576	239.367	217.727	62.755	1140.154	585.862	−10.553
3000	25.816	240.238	218.463	65.324	1140.078	566.750	−9.868
3100	26.048	241.088	219.179	67.918	1140.026	547.640	−9.228
3200	26.272	241.919	219.877	70.534	1139.997	528.531	−8.627
3300	26.486	242.731	220.557	73.172	1139.990	509.423	−8.063
3400	26.689	243.524	221.221	75.831	1140.004	490.315	−7.533
3500	26.881	244.301	221.870	78.509	1140.037	471.206	−7.032
3600	27.060	245.061	222.503	81.206	1140.089	452.096	−6.560
3700	27.228	245.804	223.123	83.921	731.060	440.772	−6.223
3800	27.384	246.533	223.730	86.652	732.380	432.909	−5.951
3900	27.528	247.246	224.323	89.397	733.660	425.011	−5.692
4000	27.660	247.944	224.905	92.157	734.899	417.081	−5.447
4100	27.781	248.629	225.476	94.929	736.098	409.121	−5.212
4200	27.890	249.300	226.035	97.712	737.258	401.132	−4.989
4300	27.989	249.957	226.584	100.507	738.379	393.115	−4.775
4400	28.078	250.602	227.122	103.310	739.462	385.073	−4.571
4500	28.157	251.234	227.651	106.122	740.507	377.007	−4.376
4600	28.227	251.853	228.170	108.941	741.517	368.918	−4.189
4700	28.289	252.461	228.681	111.767	742.491	360.808	−4.010
4800	28.343	253.057	229.182	114.599	743.431	352.677	−3.838
4900	28.390	253.642	229.676	117.435	744.339	344.527	−3.673
5000	28.430	254.216	230.161	120.276	745.215	336.358	−3.514
5100	28.464	254.779	230.638	123.121	746.061	328.173	−3.361
5200	28.493	255.332	231.107	125.969	746.879	319.971	−3.214
5300	28.516	255.875	231.570	128.819	747.669	311.753	−3.073
5400	28.535	256.408	232.025	131.672	748.434	303.521	−2.936
5500	28.550	256.932	232.473	134.526	749.175	295.275	−2.804
5600	28.561	257.447	232.914	137.382	749.893	287.016	−2.677
5700	28.569	257.952	233.349	140.238	750.589	278.744	−2.554
5800	28.575	258.449	233.778	143.096	751.266	270.460	−2.436
5900	28.578	258.938	234.200	145.953	751.925	262.165	−2.321
6000	28.579	259.418	234.616	148.811	752.566	253.858	−2.210

PREVIOUS: June 1979 (1 atm) CURRENT: March 1984 (1 bar)

EA(Ti, g) = 0.079 ± 0.014 eV
$S°(298.15\ K) = 183.715 \pm 0.001\ J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K) = 463.3 \pm 4\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = [459.833]\ kJ·mol^{-1}$

Electonic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^4F_3$	0	4
$^4F_{5/2}$	72	6
$^4F_{7/2}$	171	8
$^4F_{9/2}$	295	10

Enthalpy of Formation

$\Delta_f H°(Ti^-, g, 0\ K)$ is calculated from $\Delta_f H°(Ti, g, 0\ K)$[1] using the adopted electron affinity of EA(Ti) = 0.079 ± 0.014 eV (7.622 ± 1.351 $kJ·mol^{-1}$). This value, recommended by Hotop and Lineberger,[2] is based on a laser photodetachment electron spectrometry study.[3] Additional information on $Ti^-(g)$ may be obtained in the critical discussions of Hotop and Lineberger,[2,4] Rosenstock *et al.*[5] and Massey.[6]

$\Delta_f H°(Ti^-, g, 298.15\ K)$ is obtained from $\Delta_f H°(Ti, g, 0\ K)$ by using EA(Ti) with JANAF[1] enthalpies, $H°(0\ K) - H°(298.15\ K)$, for $Ti^-(g)$, Ti(g), and e^-(ref). $\Delta_r H°(Ti^- \rightarrow Ti + e^-, 298.15\ K)$ 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 $Ti^-(g)$ is given by Hotop and Lineberger,[2,4] Rosenstock *et al.*[5] and Massey.[6] The fine structure has been calculated via an isoelectronic extrapolation from a logarithmic plot[3] and is that recommended by Hotop and Lineberger.[2]

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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	−7.563	463.297		
100	28.077	155.897	205.362	−4.947			
200	24.629	174.264	185.851	−2.317			
250	23.533	179.634	184.094	−1.115			
298.15	22.835	183.715	183.715	0.	459.833	420.484	−73.667
300	22.813	183.856	183.715	0.042	459.790	420.240	−73.170
350	22.330	187.334	183.991	1.170	458.591	413.742	−61.748
400	21.995	190.293	184.598	2.278	457.333	407.420	−53.204
450	21.756	192.869	185.377	3.371	456.030	401.259	−46.577
500	21.580	195.151	186.243	4.454	454.691	395.245	−41.291
600	21.344	199.063	188.064	6.600	451.932	383.613	−33.396
700	21.199	202.342	189.876	8.726	449.092	372.450	−27.793
800	21.103	205.166	191.615	10.841	446.203	361.698	−23.616
900	21.037	207.647	193.261	12.948	443.241	351.311	−20.390
1000	20.990	209.861	194.812	15.049	440.142	341.261	−17.826
1100	20.955	211.860	196.273	17.146	436.846	331.531	−15.743
1200	20.928	213.682	197.649	19.240	429.366	322.230	−14.026
1300	20.907	215.356	198.947	21.332	426.399	313.422	−12.593
1400	20.890	216.905	200.175	23.422	423.351	304.845	−11.374
1500	20.877	218.346	201.339	25.510	420.211	296.489	−10.325
1600	20.866	219.693	202.445	27.597	416.965	288.346	−9.414
1700	20.857	220.958	203.497	29.683	413.600	280.410	−8.616
1800	20.849	222.150	204.500	31.769	410.103	272.676	−7.913
1900	20.843	223.277	205.459	33.853	406.461	265.139	−7.289
2000	20.837	224.346	206.377	35.937	387.974	258.253	−6.745
2100	20.832	225.362	207.257	38.021	383.255	251.883	−6.265
2200	20.828	226.331	208.102	40.104	378.536	245.737	−5.835
2300	20.825	227.257	208.915	42.186	373.816	239.807	−5.446
2400	20.821	228.143	209.698	44.269	369.096	234.082	−5.095
2500	20.819	228.993	210.453	46.351	364.376	228.553	−4.775
2600	20.816	229.810	211.182	48.432	359.655	223.213	−4.484
2700	20.814	230.595	211.886	50.514	354.934	218.055	−4.219
2800	20.812	231.352	212.568	52.595	350.213	213.072	−3.975
2900	20.810	232.082	213.228	54.676	345.492	208.257	−3.751
3000	20.809	232.788	213.869	56.757	340.770	203.605	−3.545
3100	20.807	233.470	214.490	58.838	336.049	199.111	−3.355
3200	20.806	234.131	215.094	60.919	331.327	194.769	−3.179
3300	20.805	234.771	215.680	62.999	326.605	190.575	−3.017
3400	20.804	235.392	216.251	65.080	321.884	186.523	−2.866
3500	20.803	235.995	216.806	67.160	317.162	182.611	−2.725
3600	20.802	236.581	217.348	69.240	312.439	178.834	−2.595
3700	20.801	237.151	217.875	71.320	−101.381	182.976	−2.583
3800	20.800	237.706	218.390	73.400	−104.869	190.708	−2.621
3900	20.799	238.246	218.892	75.480	−108.413	198.532	−2.659
4000	20.799	238.773	219.382	77.560	−112.010	206.448	−2.696
4100	20.798	239.286	219.862	79.640	−115.660	214.455	−2.732
4200	20.798	239.787	220.330	81.720	−119.362	222.551	−2.768
4300	20.797	240.277	220.788	83.800	−123.112	230.736	−2.803
4400	20.797	240.755	221.237	85.879	−126.910	239.009	−2.837
4500	20.796	241.222	221.676	87.959	−130.754	247.368	−2.871
4600	20.796	241.679	222.106	90.038	−134.642	255.814	−2.905
4700	20.795	242.126	222.527	92.118	−138.571	264.344	−2.938
4800	20.795	242.564	222.940	94.197	−142.540	272.959	−2.970
4900	20.794	242.993	223.345	96.277	−146.547	281.656	−3.002
5000	20.794	243.413	223.742	98.356	−150.590	290.436	−3.034
5100	20.794	243.825	224.132	100.436	−154.666	299.297	−3.065
5200	20.794	244.229	224.514	102.515	−158.774	308.238	−3.096
5300	20.793	244.625	224.890	104.594	−162.912	317.259	−3.127
5400	20.793	245.013	225.259	106.674	−167.077	326.357	−3.157
5500	20.793	245.395	225.622	108.753	−171.269	335.534	−3.187
5600	20.792	245.770	225.978	110.832	−175.485	344.786	−3.216
5700	20.792	246.138	226.329	112.912	−179.722	354.114	−3.245
5800	20.792	246.499	226.673	114.991	−183.981	363.517	−3.274
5900	20.792	246.855	227.012	117.070	−188.258	372.993	−3.302
6000	20.792	247.204	227.346	119.149	−192.552	382.542	−3.330

PREVIOUS: June 1979 (1 atm) CURRENT: March 1984 (1 bar)

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REFERENCE STATE

0	to	2190	K crystal
2190	to	3690.080	K liquid
above		3690.080	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

	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	−4.640	0.	0.	0.
100	13.119	7.185	48.695	−4.151	0.	0.	0.
200	21.876	19.558	31.133	−2.315	0.	0.	0.
298.15	24.896	28.936	28.936	0.	0.	0.	0.
300	24.928	29.090	28.936	0.046	0.	0.	0.
400	26.234	36.459	29.932	2.611	0.	0.	0.
500	26.945	42.392	31.850	5.271	0.	0.	0.
600	27.489	47.353	34.032	7.993	0.	0.	0.
700	28.033	51.630	36.247	10.768	0.	0.	0.
800	28.660	55.413	38.411	13.602	0.	0.	0.
900	29.372	58.830	40.493	16.504	0.	0.	0.
1000	30.083	61.961	42.485	19.476	0.	0.	0.
1100	30.878	64.864	44.389	22.523	0.	0.	0.
1200	31.798	67.590	46.210	25.656	0.	0.	0.
1300	32.740	70.172	47.955	28.882	0.	0.	0.
1400	33.807	72.638	49.630	32.210	0.	0.	0.
1500	34.811	75.004	51.244	35.640	0.	0.	0.
1600	35.857	77.283	52.800	39.173	0.	0.	0.
1700	37.028	79.492	54.306	42.817	0.	0.	0.
1800	38.200	81.641	55.765	46.577	0.	0.	0.
1900	39.539	83.742	57.182	50.464	0.	0.	0.
2000	40.920	85.805	58.562	54.485	0.	0.	0.
2100	42.468	87.837	59.908	58.652	0.	0.	0.
2190.000	44.141	89.653	61.093	62.547	CRYSTAL <--> LIQUID		
2190.000	46.204	100.085	61.093	85.392	TRANSITION		
2200	46.204	100.295	61.271	85.854	0.	0.	0.
2300	46.204	102.349	63.012	90.474	0.	0.	0.
2400	46.204	104.315	64.693	95.095	0.	0.	0.
2500	46.204	106.202	66.316	99.715	0.	0.	0.
2600	46.204	108.014	67.885	104.335	0.	0.	0.
2700	46.204	109.757	69.403	108.956	0.	0.	0.
2800	46.204	111.438	70.875	113.576	0.	0.	0.
2900	46.204	113.059	72.302	118.197	0.	0.	0.
3000	46.204	114.626	73.687	122.817	0.	0.	0.
3100	46.204	116.141	75.032	127.437	0.	0.	0.
3200	46.204	117.607	76.339	132.058	0.	0.	0.
3300	46.204	119.029	77.612	136.678	0.	0.	0.
3400	46.204	120.409	78.850	141.299	0.	0.	0.
3500	46.204	121.748	80.057	145.919	0.	0.	0.
3600	46.204	123.049	81.233	150.539	0.	0.	0.
3690.080	46.204	124.191	82.268	154.701	LIQUID <--> IDEAL GAS		
3690.080	29.042	245.321	82.268	601.678	FUGACITY = 1 bar		
3700	29.090	245.399	82.705	601.967	0.	0.	0.
3800	29.591	246.181	86.997	604.901	0.	0.	0.
3900	30.105	246.956	91.088	607.885	0.	0.	0.
4000	30.631	247.725	94.995	610.922	0.	0.	0.
4100	31.166	248.488	98.729	614.012	0.	0.	0.
4200	31.710	249.246	102.304	617.156	0.	0.	0.
4300	32.260	249.998	105.730	620.354	0.	0.	0.
4400	32.817	250.746	109.017	623.608	0.	0.	0.
4500	33.379	251.490	112.175	626.918	0.	0.	0.
4600	33.946	252.230	115.211	630.284	0.	0.	0.
4700	34.517	252.966	118.135	633.707	0.	0.	0.
4800	35.093	253.699	120.951	637.187	0.	0.	0.
4900	35.672	254.428	123.668	640.726	0.	0.	0.
5000	36.255	255.155	126.290	644.322	0.	0.	0.
5100	36.843	255.878	128.824	647.977	0.	0.	0.
5200	37.435	256.600	131.274	651.691	0.	0.	0.
5300	38.031	257.318	133.646	655.464	0.	0.	0.
5400	38.632	258.035	135.943	659.297	0.	0.	0.
5500	39.238	258.749	138.169	663.190	0.	0.	0.
5600	39.849	259.462	140.329	667.144	0.	0.	0.
5700	40.465	260.172	142.425	671.160	0.	0.	0.
5800	41.087	260.881	144.461	675.237	0.	0.	0.
5900	41.712	261.589	146.440	679.376	0.	0.	0.
6000	42.343	262.295	148.365	683.579	0.	0.	0.

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