Krypton (Kr) REFERENCE STATE $A_r = 83.80$ Krypton (Kr) Kr_1(ref)

0 to 6000 K Ideal Monatomic Gas

IP(Kr, g) = 112914.5 ± 0.1 cm^{-1}
$S°$(298.15 K) = 164.084 ± 0.003 $J\cdot K^{-1}\cdot mol^{-1}$

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

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
$^1S_0$	0	1

Enthalpy of Formation

Zero by definition.

Heat Capacity and Entropy

Information on the electronic energy levels and quantum weights is taken from Moore.[1,9] All predicted levels have been observed for n=4 but above that many predicted levels are missing. Our calculations indicate that any reasonable method of filling in these missing levels and cutting off the summation in the partition function[2] has no effect on the thermodynamic properties to 6000 K. This is undoubtedly a result of the high energy of these levels; the first excited level is nearly 80000 cm^{-1} above the ground state. Therefore, we list the ground state only. Extension to higher temperatures may require consideration of excited states and utilization of different fill and cutoff procedures.[2]

The thermodynamic functions at 298 15 K agree exactly with recent CODATA recommendations[3] except for two minor differences First, the entropy differs by 0.1094 $J\cdot K^{-1}\cdot mol^{-1}$ because this table uses a standard-state pressure of 1 bar, whereas the CODATA recommendations are based on 1 atm. Second, entropy differences of the order of 0.001–0.004 $J\cdot K^{-1}$ mol^{-1} for the rare gases arise due to the use of slightly different values for R; this table uses R = 8.31441 $J\cdot K^{-1}\cdot mol^{-1}$ Considering these minor changes, this table agrees within the estimated uncertainty with those by Hultgren *et al.*,[4] Hilsenrath *et al.*,[5] Gurvich *et al.*,[8] and Wagman *et al.*[12] The estimated uncertainty is due to uncertainties in the relative atomic mass and fundamental constants which are based on the 1981 scale[6] and the 1973 values,[7] respectively.

Phase Data

The triple point, 115.770 K, and boiling point, 119.800 K, are secondary fixed points of IPTS–68.[10,11] Hultgren *et al.*[4] had recommended a triple point of 115.78 K (0.7220 atm) and a boiling point of 119.86 K (1 atm) These values are provided for the convenience of the reader and have not been evaluated by the present authors. As a result of these low values, the reference state for krypton is chosen to be the ideal gas at all temperatures. This may differ from the choice of other authors.

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	−6.197	0.	0.	0
100	20.786	141.377	182.565	−4.119	0.	0.	0.
200	20.786	155.785	165.986	−2.040	0.	0.	0.
250	20.786	160.423	164.427	−1.001	0.	0.	0.
298.15	20.786	164.084	164.084	0.	0.	0.	0.
300	20.786	164.213	164.085	0.038	0.	0.	0.
350	20.786	167.417	164.338	1.078	0.	0.	0.
400	20.786	170.193	164.900	2.117	0	0.	0.
450	20.786	172.641	165.627	3.156	0.	0	0.
500	20.786	174.831	166.440	4.196	0.	0.	0.
600	20.786	178.621	168.164	6.274	0.	0.	0.
700	20.786	181.825	169.892	8.353	0.	0.	0.
800	20.786	184.600	171.561	10.431	0.	0.	0.
900	20.786	187.049	173.149	12.510	0.	0.	0.
1000	20.786	189.239	174.650	14.589	0.	0.	0.
1100	20.786	191.220	176.068	16.667	0.	0.	0.
1200	20.786	193.028	177.407	18.746	0.	0.	0.
1300	20.786	194.692	178.673	20.824	0.	0.	0.
1400	20.786	196.233	179.873	22.903	0.	0.	0.
1500	20.786	197.667	181.012	24.982	0.	0.	0.
1600	20.786	199.008	182.096	27.060	0.	0.	0.
1700	20.786	200.268	183.128	29.139	0.	0.	0.
1800	20.786	201.456	184.113	31.217	0.	0.	0
1900	20.786	202.580	185.056	33.296	0.	0.	0.
2000	20.786	203.646	185.959	35.375	0.	0.	0.
2100	20.786	204.661	186.826	37.453	0.	0.	0.
2200	20.786	205.628	187.659	39.532	0.	0.	0.
2300	20.786	206.552	188.460	41.610	0.	0.	0.
2400	20.786	207.436	189.232	43.689	0.	0.	0.
2500	20.786	208.285	189.978	45.768	0.	0.	0.
2600	20.786	209.100	190.698	47.846	0.	0.	0.
2700	20.786	209.884	191.394	49.925	0.	0.	0.
2800	20.786	210.640	192.068	52.004	0.	0.	0.
2900	20.786	211.370	192.721	54.082	0.	0.	0.
3000	20.786	212.074	193.354	56.161	0.	0.	0.
3100	20.786	212.756	193.969	58.239	0.	0.	0.
3200	20.786	213.416	194.567	60.318	0.	0.	0.
3300	20.786	214.056	195.148	62.397	0.	0.	0.
3400	20.786	214.676	195.713	64.475	0.	0.	0.
3500	20.786	215.279	196.263	66.554	0.	0.	0.
3600	20.786	215.864	196.800	68.632	0.	0.	0.
3700	20.786	216.434	197.323	70.711	0.	0.	0.
3800	20.786	216.988	197.833	72.790	0.	0.	0.
3900	20.786	217.528	198.331	74.868	0.	0.	0.
4000	20.786	218.054	198.818	76.947	0.	0.	0.
4100	20.786	218.567	199.293	79.025	0.	0.	0.
4200	20.786	219.068	199.758	81.104	0.	0.	0.
4300	20.786	219.557	200.213	83.183	0.	0.	0.
4400	20.786	220.035	200.658	85.261	0.	0.	0.
4500	20.786	220.502	201.094	87.340	0.	0.	0.
4600	20.786	220.959	201.521	89.418	0.	0.	0
4700	20.786	221.406	201.939	91.497	0.	0.	0.
4800	20.786	221.844	202.349	93.576	0.	0.	0.
4900	20.786	222.273	202.751	95.654	0.	0.	0.
5000	20.786	222.692	203.146	97.733	0.	0.	0.
5100	20.786	223.104	203.533	99.811	0.	0.	0.
5200	20.786	223.508	203.914	101.890	0.	0.	0.
5300	20.786	223.904	204.287	103.969	0.	0.	0.
5400	20.786	224.292	204.654	106.047	0.	0.	0.
5500	20.786	224.674	205.014	108.126	0.	0.	0.
5600	20.786	225.048	205.369	110.204	0.	0.	0.
5700	20.786	225.416	205.717	112.283	0.	0.	0.
5800	20.786	225.778	206.060	114.362	0.	0.	0.
5900	20.786	226.133	206.397	116.440	0.	0.	0.
6000	20.786	226.482	206.729	118.519	0.	0.	0.

PREVIOUS. March 1977 (1 atm) CURRENT: March 1982 (1 bar)

IP(Kr^+, g) = 196474.8 ± 0.1 cm^{-1}
$S°$(298.15 K) = 175.610 ± 0.003 $J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°$(0 K) = 1350.758 ± 0.012 kJ mol^{-1}
$\Delta_f H°$(298 15 K) = [1356.955] kJ·mol^{-1}

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^2P_{3/2}$	0	4
$^2P_{1/2}$	5371.00	2

Heat of Formation

The ionization limit of neutral krypton (112914.5 ± 0 1 cm^{-1}) reported by Moore[1] is adopted as $\Delta_f H°$(0 K) for Kr^+(g). 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 latest CODATA fundamental constants.[2] The uncertainty in the ionization limit is estimated to be ±0.1 cm^{-1} which corresponds to an uncertainty of ±0.012 kJ·mol^{-1} in the heat of formation. Rosenstock *et al*[9] and Levin and Lias[11] have summarized additional ionization potential and appearance potential data. The recent spectroscopic study by Yoshino *et al.*[12] is in agreement with our adopted value. Gurvich *et al.*[8] and Wagman *et al.*[10] adopted the same ionization potential, but the use of slightly different fundamental constants by Wagman *et al.*[10] resulted in a heat of formation difference of 0.012 kJ·mol^{-1}. However, the study by Chaghtai *et al.*[13] suggests an ionization potential which is larger by 10 cm^{-1}.

$\Delta_f H°$(Kr^+, g, 298 15 K) is obtained from $\Delta_f H°$(Kr, g, 0 K) by using IP(Kr) with JANAF[3] enthalpies $H°$(0 K)–$H°$(298 15 K) for Kr^+(g), Kr(r), and e^-(r). $\Delta_r H°$(Kr → $Kr^+ + e^-$, 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.*[9] $\Delta_f H°$(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[4] is incomplete because many theoretically predicted levels have not been observed. Our calculations indicate that any reasonable method of filling in these missing levels and cutting off the summation in the partition function[5] has no effect on the thermodynamic functions to 6000 K. This is a result of the high energy of all levels other than the ground state and the $^2P_{1/2}$ level, the next lowest level is over 109000 cm^{-1} above the ground state. Since inclusion of these upper levels has no effect on the thermodynamic functions (to 6000 K) we list only the ground state and the $^2P_{1/2}$ state, with the energy of the latter state taken from a more recent study by Moore.[1] The reported uncertainty in $S°$(298 15 K) is due to uncertainties in the relative ionic mass and fundamental constants. Extension of these calculations above 6000 K may require consideration of the higher excited states and use of different fill and cutoff procedures.[5]

The thermodynamic functions reported here agree with those of Green *et al*,[6] Hilsenrath *et al.*,[7] and Gurvich *et al.*[8] except for one or two minor changes. First, the entropy differs by 0.1094 $J \cdot K^{-1} \cdot mol^{-1}$ because this table uses a standard–state pressure of 1 bar, whereas the cited references used a pressure of 1 atm Second, smaller differences arise from the use of slightly different values for the fundamental constants, the relative ionic mass, and the position of the $^2P_{1/2}$ electronic level.

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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	−6 197	1350 758		
100	20.786	152.903	194.091	−4.119			
200	20.786	167.311	177.512	−2.040			
250	20.786	171.949	175.953	−1.001			
298 15	20.786	175 610	175.610	0	1356.955	1347.264	−236.035
300	20.786	175.739	175.611	0.038	1356.994	1347.204	−234.569
350	20.786	178.943	175.864	1.078	1358.033	1345.490	−200.803
400	20.786	181 719	176.426	2.117	1359.072	1343.627	−175.460
450	20 786	184.167	177.153	3 156	1360.111	1341.634	−155.733
500	20 786	186.357	177.966	4.196	1361.151	1339.525	−139.939
600	20.788	190.147	179.690	6.274	1363.229	1335.005	−116.222
700	20.794	193.352	181.418	8.353	1365.308	1330 136	−99.256
800	20.811	196.129	183.087	10.434	1367.389	1324.970	−86.512
900	20.843	198.582	184.675	12.516	1369.471	1319.542	−76.584
1000	20 895	200.781	186.178	14.603	1371.558	1313.883	−68.630
1100	20.968	202.776	187.598	16.696	1373.651	1308.014	−62.112
1200	21.061	204.604	188.940	18.797	1375.752	1301.954	−56.673
1300	21.170	206.294	190.210	20.909	1377.864	1295.719	−52.063
1400	21.291	207.867	191.416	23.032	1379.987	1289.321	−48.105
1500	21.421	209.340	192.562	25.167	1382.122	1282.770	−44.670
1600	21.555	210.727	193.655	27.316	1384.271	1276.077	−41.660
1700	21.688	212.038	194.698	29.478	1386.433	1269.248	−38.999
1800	21.819	213.281	195.696	31.653	1388.609	1262.292	−36.631
1900	21.944	214.464	196.653	33.842	1390 797	1255.215	−34.508
2000	22.062	215.593	197.572	36.042	1392.997	1248.022	−32.595
2100	22.171	216.672	198.456	38.254	1395.209	1240.719	−30.861
2200	22.271	217.706	199.308	40 476	1397.431	1233.311	−29.283
2300	22.361	218.698	200.129	42.707	1399.663	1225.801	−27.839
2400	22.441	219.651	200.923	44 948	1401.903	1218.194	−26.513
2500	22.512	220.569	201.691	47.195	1404 151	1210 493	−25.292
2600	22.573	221.453	202.434	49.450	1406.405	1202.702	−24.163
2700	22.626	222.306	203.154	51.710	1408.665	1194.824	−23.115
2800	22.669	223.130	203.853	53.975	1410.930	1186.863	−22.141
2900	22.705	223.926	204.531	56.243	1413.199	1178.821	−21.233
3000	22.734	224.696	205.191	58.515	1415.471	1170.700	−20.384
3100	22.756	225.442	205.832	60.790	1417.745	1162.503	−19.588
3200	22.771	226.164	206.456	63.066	1420.021	1154.233	−18.841
3300	22.782	226.865	207.064	65.344	1422.299	1145.892	−18.138
3400	22.787	227.546	207.657	67.623	1424.578	1137.482	−17.475
3500	22.788	228.206	208.234	69.901	1426.856	1129.005	−16.849
3600	22.785	228.848	208.798	72.180	1429.135	1120.463	−16.257
3700	22.778	229.472	209.348	74 458	1431.413	1111.857	−15.697
3800	22.768	230.080	209.886	76.735	1433.690	1103 190	−15.164
3900	22.755	230.671	210.411	79.012	1435.967	1094.463	−14.659
4000	22.740	231.247	210.925	81.286	1438.241	1085.677	−14.177
4100	22.723	231.808	211.428	83.560	1440.515	1076.835	−13.719
4200	22.704	232.355	211.919	85.831	1442.786	1067 938	−13.282
4300	22.684	232.889	212.401	88.100	1445.056	1058.986	−12.864
4400	22.662	233.411	212.873	90.368	1447.323	1049.981	−12.465
4500	22.640	233.920	213.335	92.633	1449.588	1040.925	−12.083
4600	22.616	234.417	213.788	94.896	1451.851	1031.819	−11.717
4700	22.591	234.903	214.232	97.156	1454.111	1022.663	−11.366
4800	22.566	235.378	214.667	99.414	1456.369	1013.460	−11.029
4900	22.541	235.844	215.095	101.669	1458.624	1004.209	−10.705
5000	22.515	236.299	215.514	103.922	1460.877	994.912	−10.394
5100	22.489	236.744	215.926	106.172	1463.127	985.571	−10.094
5200	22.463	237.181	216.331	108 420	1465.375	976.185	−9.806
5300	22.436	237.608	216.728	110.665	1467.620	966.756	−9.528
5400	22.410	238.027	217.119	112.907	1469.862	957.285	−9.260
5500	22.384	238 438	217.503	115.147	1472.102	947.772	−9.001
5600	22.357	238.841	217.880	117.384	1474.339	938.219	−8.751
5700	22.332	239.237	218.251	119.618	1476.573	928.625	−8.510
5800	22.306	239.625	218.617	121.850	1478.805	918.992	−8.276
5900	22.280	240.006	218.976	124.079	1481.034	909.321	−8.051
6000	22 255	240.380	219.329	126.306	1483.261	899.613	−7.832

PREVIOUS March 1977 (1 atm) — CURRENT March 1982 (1 bar)