0 to 6000 K Ideal Monatomic Gas

IP(Ar, g) = 12710 ± 0.1 cm^{-1}
$S°(298.15\ K) = 154.845 \pm 0.003\ J \cdot K^{-1} \cdot mol^{-1}$

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

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=3 and 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 over 93000 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 $J \cdot K^{-1} \cdot mol^{-1}$ 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] McBride *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, 83.798 K, and boiling point, 87.294 K, are a defining fixed point and a secondary reference point, respectively of IPTS-68.[10,11] Hultgren *et al.*[4] had recommended a triple point of 83.81 K (0.6801 atm) and a boiling point of 87.30 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 argon is chosen to be the ideal gas at all temperatures. This may differ from the choice of other authors.

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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
	$J \cdot K^{-1} \cdot mol^{-1}$			$kJ \cdot mol^{-1}$			
0	0.	0.	INFINITE	−6.197	0.	0.	0.
100	20.786	132.137	173.325	−4.119	0.	0.	0.
200	20.786	146.545	156.746	−2.040	0.	0.	0.
250	20.786	151.183	155.187	−1.001	0.	0.	0.
298.15	20.786	154.845	154.845	0.	0.	0.	0.
300	20.786	154.973	154.845	0.038	0.	0.	0.
350	20.786	158.177	155.098	1.078	0.	0.	0.
400	20.786	160.953	155.660	2.117	0.	0.	0.
450	20.786	163.401	156.387	3.156	0.	0.	0.
500	20.786	165.591	157.200	4.196	0.	0.	0.
600	20.786	169.381	158.924	6.274	0.	0.	0.
700	20.786	172.585	160.653	8.353	0.	0.	0.
800	20.786	175.361	162.321	10.431	0.	0.	0.
900	20.786	177.809	163.909	12.510	0.	0.	0.
1000	20.786	179.999	165.410	14.589	0.	0.	0.
1100	20.786	181.980	166.828	16.667	0.	0.	0.
1200	20.786	183.789	168.167	18.746	0.	0.	0.
1300	20.786	185.453	169.434	20.824	0.	0.	0.
1400	20.786	186.993	170.634	22.903	0.	0.	0.
1500	20.786	188.427	171.773	24.982	0.	0.	0.
1600	20.786	189.769	172.856	27.060	0.	0.	0.
1700	20.786	191.029	173.888	29.139	0.	0.	0.
1800	20.786	192.217	174.874	31.217	0.	0.	0.
1900	20.786	193.341	175.816	33.296	0.	0.	0.
2000	20.786	194.407	176.719	35.375	0.	0.	0.
2100	20.786	195.421	177.586	37.453	0.	0.	0.
2200	20.786	196.388	178.419	39.532	0.	0.	0.
2300	20.786	197.312	179.220	41.610	0.	0.	0.
2400	20.786	198.197	179.993	43.689	0.	0.	0.
2500	20.786	199.045	180.738	45.768	0.	0.	0.
2600	20.786	199.860	181.458	47.846	0.	0.	0.
2700	20.786	200.645	182.154	49.925	0.	0.	0.
2800	20.786	201.401	182.828	52.004	0.	0.	0.
2900	20.786	202.130	183.481	54.082	0.	0.	0.
3000	20.786	202.835	184.115	56.161	0.	0.	0.
3100	20.786	203.516	184.730	58.239	0.	0.	0.
3200	20.786	204.176	185.327	60.318	0.	0.	0.
3300	20.786	204.816	185.908	62.397	0.	0.	0.
3400	20.786	205.436	186.473	64.475	0.	0.	0.
3500	20.786	206.039	187.024	66.554	0.	0.	0.
3600	20.786	206.625	187.560	68.632	0.	0.	0.
3700	20.786	207.194	188.083	70.711	0.	0.	0.
3800	20.786	207.748	188.593	72.790	0.	0.	0.
3900	20.786	208.288	189.091	74.868	0.	0.	0.
4000	20.786	208.815	189.578	76.947	0.	0.	0.
4100	20.786	209.328	190.053	79.025	0.	0.	0.
4200	20.786	209.829	190.518	81.104	0.	0.	0.
4300	20.786	210.318	190.973	83.183	0.	0.	0.
4400	20.786	210.796	191.418	85.261	0.	0.	0.
4500	20.786	211.263	191.854	87.340	0.	0.	0.
4600	20.786	211.720	192.281	89.418	0.	0.	0.
4700	20.786	212.167	192.699	91.497	0.	0.	0.
4800	20.786	212.604	193.109	93.576	0.	0.	0.
4900	20.786	213.033	193.512	95.654	0.	0.	0.
5000	20.786	213.453	193.906	97.733	0.	0.	0.
5100	20.786	213.864	194.294	99.811	0.	0.	0.
5200	20.786	214.268	194.674	101.890	0.	0.	0.
5300	20.786	214.664	195.047	103.969	0.	0.	0.
5400	20.786	215.053	195.414	106.047	0.	0.	0.
5500	20.786	215.434	195.775	108.126	0.	0.	0.
5600	20.786	215.808	196.129	110.204	0.	0.	0.
5700	20.786	216.176	196.478	112.283	0.	0.	0.
5800	20.786	216.538	196.820	114.362	0.	0.	0.
5900	20.786	216.893	197.158	116.440	0.	0.	0.
6000	20.786	217.243	197.489	118.519	0.	0.	0.

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

IP(Ar^+, g) = 222848.2 ± 0.1 cm^{-1}
8.15 K) = 166.404 ± 0.003 $J \cdot K^{-1} \cdot mol^{-1}$

$H°(0\ K) = 1520.573 \pm 0.001\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = [1526.778]\ kJ \cdot mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^2P_{3/2}$	0	4
$^2P_{1/2}$	1431.41	2

Enthalpy of Formation

The ionization limit of neutral argon (127109.9 ± 0.1 cm^{-1}) reported by Moore[1] is adopted as $\Delta_f H°(0\ K)$ for $Ar^+(g)$. The ionization limit is converted from cm^{-1} to $kJ \cdot mol^{-1}$ using the factor, 1 cm^{-1} = 0.01196266 $kJ \cdot mol^{-1}$, which is derived from the latest CODATA fundamental constants.[2] The uncertainty in the ionization limit corresponds to an uncertainty of ±0.001 $kJ \cdot mol^{-1}$ in the heat of formation Rosenstock *et al.*[9] and Levin and Lias[11] have summarized additional ionization potential and appearance potential data. A recent atomic spectroscopic study by Minnhagen[12] yielded an ionization potential within 0.13 cm^{-1} of 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 0.015 $kJ \cdot mol^{-1}$.

$\Delta_f H°(Ar^+, g, 298.15\ K)$ is obtained from $\Delta_f H°(Ar, g, 0\ K)$ by using IP(Ar) with JANAF[3] enthalpies $H°(0\ K) - H°(298.15\ K)$ for $Ar^+(r)$, Ar(g), and $e^-(r)$. $\Delta_r H°(Ar \rightarrow Ar^+ + e^-, 298.15\ K)$ 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 $kJ \cdot mol^{-1}$ 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 108000 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 $J \cdot K^{-1}$ 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

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
0	0.	0.	INFINITE	−6.206	1520.573		
100	20.786	143.663	184.937	−4.127			
200	20.801	158.073	168.315	−2.048			
250	20.861	162.720	166.748	−1.007			
298.15	20.984	166.404	166.404	0.	1526.778	1517.077	−265.786
300	20.990	166.533	166.404	0.039	1526.817	1517.017	−264.136
350	21.185	169.783	166.660	1.093	1527.871	1515.300	−226.146
400	21.422	172.627	167.232	2.158	1528.936	1513.432	−197.634
450	21.673	175.165	167.975	3.235	1530.014	1511.429	−175.442
500	21.915	177.461	168.810	4.325	1531.104	1509.306	−157.676
600	22.318	181.494	170.597	6.538	1533.316	1504.740	−130.999
700	22.588	184.956	172.407	8.784	1535.563	1499.800	−111.916
800	22.734	187.983	174.169	11.051	1537.830	1494.536	−97.583
900	22.786	190.665	175.856	13.328	1540.106	1488.988	−86.419
1000	22.773	193.065	177.459	15.606	1542.385	1483.186	−77.474
1100	22.718	195.234	178.978	17.881	1544.660	1477.156	−70.144
1200	22.639	197.207	180.416	20.149	1546.928	1470.919	−64.027
1300	22.546	199.015	181.778	22.409	1549.187	1464.493	−58.844
1400	22.449	200.683	183.070	24.658	1551.437	1457.893	−54.395
1500	22.350	202.228	184.296	26.898	1553.677	1451.134	−50.533
1600	22.254	203.668	185.462	29.129	1555.907	1444.225	−47.149
1700	22.162	205.014	186.573	31.349	1558.128	1437.176	−44.159
1800	22.076	206.278	187.633	33.561	1560.340	1429.998	−41.497
1900	21.995	207.470	188.646	35.765	1562.543	1422.696	−39.113
2000	21.919	208.596	189.616	37.960	1564.739	1415.279	−36.963
2100	21.849	209.664	190.545	40.149	1566.927	1407.752	−35.016
2200	21.785	210.679	191.437	42.330	1569.109	1400.121	−33.243
2300	21.725	211.646	192.295	44.506	1571.284	1392.391	−31.622
2400	21.670	212.569	193.121	46.675	1573.454	1384.567	−30.134
2500	21.619	213.453	193.917	48.840	1575.618	1376.652	−28.764
2600	21.571	214.299	194.684	50.999	1577.778	1368.651	−27.497
2700	21.528	215.113	195.426	53.154	1579.933	1360.567	−26.322
2800	21.487	215.895	196.143	55.305	1582.083	1352.403	−25.229
2900	21.450	216.648	196.837	57.452	1584.230	1344.162	−24.211
3000	21.415	217.375	197.510	59.595	1586.374	1335.847	−23.259
3100	21.383	218.077	198.162	61.735	1588.513	1327.461	−22.368
3200	21.353	218.755	198.795	63.872	1590.650	1319.006	−21.531
3300	21.326	219.412	199.410	66.006	1592.784	1310.484	−20.743
3400	21.300	220.048	200.008	68.137	1594.915	1301.897	−20.001
3500	21.276	220.665	200.589	70.266	1597.044	1293.248	−19.301
3600	21.253	221.264	201.155	72.392	1599.171	1284.538	−18.638
3700	21.232	221.846	201.706	74.516	1601.295	1275.769	−18.011
3800	21.212	222.412	202.244	76.639	1603.417	1266.943	−17.415
3900	21.194	222.963	202.768	78.759	1605.537	1258.060	−16.850
4000	21 176	223.499	203.280	80.877	1607.656	1249.124	−16.312
4100	21.160	224.022	203.779	82.994	1609.773	1240.134	−15.800
4200	21.145	224.532	204.267	85.110	1611.888	1231.093	−15.311
4300	21.130	225.029	204.744	87.223	1614.002	1222.002	−14.844
4400	21.117	225.515	205.211	89.336	1616.114	1212.861	−14.398
4500	21.104	225.989	205.667	91.447	1618.225	1203.672	−13.972
4600	21.092	226.453	206.114	93.556	1620.335	1194.437	−13.563
4700	21.080	226.906	206.552	95.665	1622.443	1185.155	−13.172
4800	21.070	227.350	206.981	97.773	1624.551	1175.829	−12.796
4900	21.059	227.784	207.401	99.879	1626.657	1166.459	−12.435
5000	21.050	228.210	207.813	101.984	1628.763	1157.046	−12.088
5100	21.040	228.626	208.217	104.089	1630.867	1147.590	−11.754
5200	21.032	229.035	208.613	106.193	1632.971	1138.094	−11.432
5300	21.023	229.435	209.002	108.295	1635.074	1128.557	−11.123
5400	21.015	229.828	209.384	110.397	1637.176	1118.980	−10.824
5500	21.008	230.214	209.759	112.498	1639.277	1109.365	−10.536
5600	21.001	230.592	210.128	114.599	1641.377	1099.711	−10.258
5700	20.994	230.964	210.490	116.699	1643.477	1090.020	−9.989
5800	20.987	231.329	210.847	118.798	1645.576	1080.292	−9.729
5900	20.981	231.688	211.197	120.896	1647.675	1070.527	−9.478
6000	20.975	232.040	211.541	122.994	1649.772	1060.728	−9.234

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