0 to 6000 K Ideal Monatomic Gas

IP(He, g) = 198310.76 ± 0.02 cm^{-1}
$S°(298.15\ K) = 126.152 \pm 0.002\ J \cdot K^{-1} \cdot mol^{-1}$

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

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
$^1S_0$	0	1

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Information on the electronic energy levels and quantum weights is taken from Moore[1] and Martin.[9] All predicted levels have been observed through 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 over 159000 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

The thermodynamic functions reported here are calculated assuming that helium gas obeys Boltzmann statistics. In fact helium is a Bose–Einstein gas.[4] However, the differences in thermal properties between the two are very small except at extremely low temperature.[10,11] At 298.15 K the difference in $C_p°$ amounts to only 0.004 $J \cdot K^{-1}$ mol^{-1} and will be less at higher temperatures. Since $C_p°$ is the most sensitive of the thermodynamic properties, the differences are well within the stated uncertainty. At temperatures below approximately 50 K the differences may become significant and Bose–Einstein statistics should be used.

Phase Data

The boiling point, 4.215 K (1 atm), is taken from Hultgren *et al.* This value should prove reasonably accurate, although it has not been evaluated by the present authors, and is furnished for the convenience of the reader. As a result of this low value, the reference state for helium 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	103.445	144.632	−4.119	0.	0.	0.
200	20.786	117.853	128.053	−2.040	0.	0.	0.
250	20.786	122.491	126.494	−1.001	0.	0.	0.
298.15	20.786	126.152	126.152	0.	0.	0.	0.
300	20.786	126.281	126.152	0.038	0.	0.	0.
350	20.786	129.485	126.405	1.078	0.	0.	0.
400	20.786	132.260	126.968	2.117	0.	0.	0.
450	20.786	134.709	127.694	3.156	0.	0.	0.
500	20.786	136.899	128.507	4.196	0.	0.	0.
600	20.786	140.688	130.231	6.274	0.	0.	0.
700	20.786	143.893	131.960	8.353	0.	0.	0.
800	20.786	146.668	133.629	10.431	0.	0.	0.
900	20.786	149.116	135.216	12.510	0.	0.	0.
1000	20.786	151.306	136.718	14.589	0.	0.	0.
1100	20.786	153.288	138.135	16.667	0.	0.	0.
1200	20.786	155.096	139.475	18.746	0.	0.	0.
1300	20.786	156.760	140.741	20.824	0.	0	0.
1400	20.786	158.300	141.941	22.903	0.	0.	0
1500	20.786	159.734	143.080	24.982	0.	0.	0.
1600	20.786	161.076	144.163	27.060	0.	0.	0.
1700	20.786	162.336	145.196	29.139	0.	0.	0
1800	20.786	163.524	146.181	31.217	0.	0.	0.
1900	20.786	164.648	147.124	33.296	0.	0.	0
2000	20.786	165.714	148.027	35.375	0	0.	0.
2100	20.786	166.728	148.893	37.453	0.	0.	0.
2200	20.786	167.695	149.726	39.532	0.	0.	0.
2300	20.786	168.619	150.528	41.610	0.	0.	0.
2400	20.786	169.504	151.300	43.689	0.	0.	0.
2500	20.786	170.352	152.045	45.768	0.	0.	0.
2600	20.786	171.168	152.765	47.846	0.	0.	0.
2700	20.786	171.952	153.461	49.925	0.	0	0.
2800	20.786	172.708	154.135	52.004	0.	0.	0
2900	20.786	173.438	154.789	54.082	0.	0.	0.
3000	20.786	174.142	155.422	56.161	0.	0.	0.
3100	20.786	174.824	156.037	58.239	0.	0.	0.
3200	20.786	175.484	156.634	60.318	0.	0.	0.
3300	20.786	176.123	157.215	62.397	0.	0.	0.
3400	20.786	176.744	157.781	64.475	0.	0.	0.
3500	20.786	177.346	158.331	66.554	0.	0.	0.
3600	20.786	177.932	158.867	68.632	0.	0.	0.
3700	20.786	178.501	159.390	70.711	0.	0.	0.
3800	20.786	179.056	159.901	72.790	0.	0.	0.
3900	20.786	179.596	160.399	74.868	0.	0.	0.
4000	20.786	180.122	160.885	76.947	0.	0.	0.
4100	20.786	180.635	161.361	79.025	0.	0.	0.
4200	20.786	181.136	161.826	81.104	0	0.	0.
4300	20.786	181.625	162.280	83.183	0.	0.	0.
4400	20.786	182.103	162.726	85.261	0.	0.	0.
4500	20.786	182.570	163.161	87.340	0.	0.	0.
4600	20.786	183.027	163.588	89.418	0.	0.	0.
4700	20.786	183.474	164.007	91.497	0.	0.	0.
4800	20.786	183.912	164.417	93.576	0.	0.	0.
4900	20.786	184.340	164.819	95.654	0.	0.	0.
5000	20.786	184.760	165.214	97.733	0.	0.	0.
5100	20.786	185.172	165.601	99.811	0.	0.	0.
5200	20.786	185.575	165.981	101.890	0.	0.	0.
5300	20.786	185.971	166.355	103.969	0.	0.	0.
5400	20.786	186.360	166.722	106.047	0.	0.	0.
5500	20.786	186.741	167.082	108.126	0.	0.	0.
5600	20.786	187.116	167.437	110.204	0.	0.	0.
5700	20.786	187.484	167.785	112.283	0.	0.	0.
5800	20.786	187.845	168.128	114.362	0.	0.	0.
5900	20.786	188.201	168.465	116.440	0.	0.	0.
6000	20.786	188.550	168.797	118.519	0.	0.	0.

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

IP(He^+, g) = 438908.85 ± 0.02 cm^{-1}
$S°$(298.15 K) = 131.913 ± 0.002 $J·K^{-1}·mol^{-1}$

$\Delta_f H°$(0 K) = 2372.324 ± 0.001 $kJ·mol^{-1}$
$\Delta_f H°$(298.15 K) = [2378.522] $kJ·mol^{-1}$

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

Heat of Formation

The ionization limit of neutral helium (198310.76 ± 0.02 cm^{-1}) reported by Moore[1] and Martin,[10] is adopted as $\Delta_f H°$(0 K) for He^+(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 corresponds to an uncertainty of less than 0.001 $kJ·mol^{-1}$ in the heat of formation. Rosenstock *et al.*[9] have summarized additional ionization potential and appearance potential data. Gurvich *et al.*[8] and Wagman *et al.*[11] adopted the same ionization potential, but the use of slightly different fundamental constants by Wagman *et al.*[11] resulted in a heat of formation difference of 0.021 $kJ·mol^{-1}$.

$\Delta_f H°$(He^+, g, 298.15 K) is obtained from $\Delta_f H°$(He, g, 0 K) by using IP(He) with JANAF[3] enthalpies $H°$(0 K)–$H°$(298.15 K) for He^+(g), He(r), and e^-(r) $\Delta_r H°$($He \rightarrow He^+ + e^-$, 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 complete to n=14. Our calculations indicate that any reasonable method of including these 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 these levels; the first excited level is over 329000 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. 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 differences. First, the entropy differs by 0.1094 $J·K^{-1}·mol^{-1}$ 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 and the relative ionic mass.

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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	−6.197	2372.324		
100	20.786	109.206	150.394	−4.119			
200	20.786	123.614	133.815	−2.040			
250	20.786	128.252	132.256	−1.001			
298.15	20.786	131.913	131.913	0.	2378.522	2370.549	−415.310
300	20.786	132.042	131.914	0.038	2378.560	2370.499	−412.741
350	20.786	135.246	132.167	1.078	2379.599	2369.074	−353.565
400	20.786	138.022	132.729	2.117	2380.639	2367.499	−309.164
450	20.786	140.470	133.456	3.156	2381.678	2365.794	−274.614
500	20.786	142.660	134.269	4.196	2382.717	2363.974	−246.963
600	20.786	146.450	135.993	6.274	2384.796	2360.030	−205.459
700	20.786	149.654	137.721	8.353	2386.874	2355.738	−175.787
800	20.786	152.430	139.390	10.431	2388.953	2351.148	−153.514
900	20.786	154.878	140.978	12.510	2391.032	2346.298	−136.176
1000	20.786	157.068	142.479	14.589	2393.110	2341.216	−122.293
1100	20.786	159.049	143.897	16.667	2395.189	2335.926	−110.924
1200	20.786	160.858	145.236	18.746	2397.267	2330.446	−101.442
1300	20.786	162.521	146.502	20.824	2399.346	2324.794	−93.411
1400	20.786	164.062	147.702	22.903	2401.425	2318.981	−86.522
1500	20.786	165.496	148.841	24.982	2403.503	2313.020	−80.547
1600	20.786	166.837	149.925	27.060	2405.582	2306.920	−75.313
1700	20.786	168.097	150.957	29.139	2407.660	2300.690	−70.692
1800	20.786	169.286	151.943	31.217	2409.739	2294.337	−66.580
1900	20.786	170.409	152.885	33.296	2411.818	2287.869	−62.898
2000	20.786	171.476	153.788	35.375	2413.896	2281.292	−59.581
2100	20.786	172.490	154.655	37.453	2415.975	2274.611	−56.578
2200	20.786	173.457	155.488	39.532	2418.053	2267.830	−53.845
2300	20.786	174.381	156.289	41.610	2420.132	2260.955	−51.348
2400	20.786	175.265	157.062	43.689	2422.211	2253.990	−49.057
2500	20.786	176.114	157.807	45.768	2424.289	2246.938	−46.947
2600	20.786	176.929	158.527	47.846	2426.368	2239.803	−44.998
2700	20.786	177.714	159.223	49.925	2428.446	2232.588	−43.192
2800	20.786	178.469	159.897	52.004	2430.525	2225.296	−41.513
2900	20.786	179.199	160.550	54.082	2432.604	2217.930	−39.949
3000	20.786	179.904	161.183	56.161	2434.682	2210.492	−38.488
3100	20.786	180.585	161.798	58.239	2436.761	2202.985	−37.120
3200	20.786	181.245	162.396	60.318	2438.839	2195.410	−35.836
3300	20.786	181.885	162.977	62.397	2440.918	2187.771	−34.630
3400	20.786	182.505	163.542	64.475	2442.997	2180.069	−33.493
3500	20.786	183.108	164.092	66.554	2445.075	2172.305	−32.420
3600	20.786	183.693	164.629	68.632	2447.154	2164.482	−31.406
3700	20.786	184.263	165.152	70.711	2449.232	2156.602	−30.446
3800	20.786	184.817	165.662	72.790	2451.311	2148.665	−29.535
3900	20.786	185.357	166.160	74.868	2453.390	2140.673	−28.671
4000	20.786	185.883	166.647	76.947	2455.468	2132.629	−27.849
4100	20.786	186.397	167.122	79.025	2457.547	2124.532	−27.067
4200	20.786	186.898	167.587	81.104	2459.625	2116.384	−26.321
4300	20.786	187.387	168.042	83.183	2461.704	2108.187	−25.609
4400	20.786	187.864	168.487	85.261	2463.783	2099.942	−24.929
4500	20.786	188.332	168.923	87.340	2465.861	2091.650	−24.279
4600	20.786	188.788	169.350	89.418	2467.940	2083.311	−23.657
4700	20.786	189.235	169.768	91.497	2470.018	2074.927	−23.060
4800	20.786	189.673	170.178	93.576	2472.097	2066.499	−22.488
4900	20.786	190.102	170.580	95.654	2474.176	2058.027	−21.939
5000	20.786	190.522	170.975	97.733	2476.254	2049.513	−21.411
5100	20.786	190.933	171.362	99.811	2478.333	2040.958	−20.904
5200	20.786	191.337	171.743	101.890	2480.411	2032.362	−20.415
5300	20.786	191.733	172.116	103.969	2482.490	2023.725	−19.945
5400	20.786	192.121	172.483	106.047	2484.569	2015.050	−19.492
5500	20.786	192.503	172.844	108.126	2486.647	2006.336	−19.055
5600	20.786	192.877	173.198	110.204	2488.726	1997.584	−18.633
5700	20.786	193.245	173.546	112.283	2490.804	1988.796	−18.225
5800	20.786	193.607	173.889	114.362	2492.883	1979.970	−17.832
5900	20.786	193.962	174.226	116.440	2494.962	1971.109	−17.451
6000	20.786	194.311	174.558	118.519	2497.040	1962.213	−17.083

PREVIOUS: March 1977 (1 Atm) CURRENT March 1982 (1 Bar)