0 to 6000 K Ideal Monatomic Gas

IP(Ne, g) = 173929.70 ± 0.1 cm^{-1}
$S°(298.15\ K) = 146.327 \pm 0.003\ J \cdot K^{-1} \cdot mol^{-1}$

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

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^1S_0$	0	1

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Information on the electronic energy levels and quantum weights is taken from Moore.[1] All predicted levels have been observed for n=2 and 3 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 134000 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, 24.561 K, and boiling point, 27.102 K, are a secondary reference point and a defining fixed-point, respectively, of IPTS-68.[10,11] Hultgren *et al.*[4] had recommended a triple point of 24.533 K (0.4277 atm) and a boiling point of 27.096 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 neon 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

	$J \cdot K^{-1} \cdot mol^{-1}$			$kJ \cdot mol^{-1}$			
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	−6.197	0.	0.	0.
100	20.786	123.620	164.808	−4.119	0.	0.	0.
200	20.786	138.028	148.229	−2.040	0.	0.	0.
250	20.786	142.666	146.670	−1.001	0.	0.	0.
298.15	20.786	146.327	146.327	0.	0.	0.	0.
300	20.786	146.456	146.328	0.038	0.	0.	0.
350	20.786	149.660	146.581	1.078	0.	0.	0.
400	20.786	152.436	147.143	2.117	0.	0.	0.
450	20.786	154.884	147.870	3.156	0.	0.	0
500	20.786	157.074	148.683	4.196	0.	0.	0.
600	20.786	160.864	150.407	6.274	0.	0.	0.
700	20.786	164.068	152.135	8.353	0.	0.	0.
800	20.786	166.843	153.804	10.431	0.	0.	0.
900	20.786	169.292	155.392	12.510	0.	0.	0.
1000	20.786	171.482	156.893	14.589	0.	0	0.
1100	20.786	173.463	158.311	16.667	0.	0.	0.
1200	20.786	175.271	159.650	18.746	0.	0.	0.
1300	20.786	176.935	160.916	20.824	0.	0.	0.
1400	20.786	178.476	162.116	22.903	0.	0.	0.
1500	20.786	179.910	163.255	24.982	0.	0.	0.
1600	20.786	181.251	164.339	27.060	0.	0.	0.
1700	20.786	182.511	165.371	29.139	0	0.	0.
1800	20.786	183.699	166.356	31.217	0.	0.	0.
1900	20.786	184.823	167.299	33.296	0.	0.	0.
2000	20.786	185.889	168.202	35.375	0.	0.	0.
2100	20.786	186.904	169.069	37.453	0.	0.	0.
2200	20.786	187.871	169.902	39.532	0.	0.	0.
2300	20.786	188.795	170.703	41.610	0.	0.	0.
2400	20.786	189.679	171.475	43.689	0.	0.	0.
2500	20.786	190.528	172.221	45.768	0.	0.	0.
2600	20.786	191.343	172.941	47.846	0.	0.	0.
2700	20.786	192.127	173.637	49.925	0.	0.	0.
2800	20.786	192.883	174.311	52.004	0.	0.	0.
2900	20.786	193.613	174.964	54.082	0.	0.	0.
3000	20.786	194.317	175.597	56.161	0.	0.	0.
3100	20.786	194.999	176.212	58.239	0.	0.	0.
3200	20.786	195.659	176.810	60.318	0.	0.	0.
3300	20.786	196.299	177.391	62.397	0.	0.	0.
3400	20.786	196.919	177.956	64.475	0.	0.	0.
3500	20.786	197.522	178.506	66.554	0.	0.	0.
3600	20.786	198.107	179.043	68.632	0.	0.	0.
3700	20.786	198.677	179.566	70.711	0.	0.	0.
3800	20.786	199.231	180.076	72.790	0.	0.	0.
3900	20.786	199.771	180.574	74.868	0.	0.	0.
4000	20.786	200.297	181.061	76.947	0.	0.	0.
4100	20.786	200.811	181.536	79.025	0.	0.	0.
4200	20.786	201.311	182.001	81.104	0.	0.	0.
4300	20.786	201.801	182.456	83.183	0.	0.	0.
4400	20.786	202.278	182.901	85.261	0.	0.	0.
4500	20.786	202.745	183.337	87.340	0.	0	0.
4600	20.786	203.202	183.764	89.418	0.	0.	0.
4700	20.786	203.649	184.182	91.497	0.	0.	0.
4800	20.786	204.087	184.592	93.576	0.	0.	0.
4900	20.786	204.516	184.994	95.654	0.	0.	0.
5000	20.786	204.936	185.389	97.733	0.	0.	0.
5100	20.786	205.347	185.776	99.811	0.	0.	0.
5200	20.786	205.751	186.157	101.890	0.	0.	0.
5300	20.786	206.147	186.530	103.969	0.	0.	0.
5400	20.786	206.535	186.897	106.047	0.	0.	0.
5500	20.786	206.917	187.257	108.126	0.	0.	0.
5600	20.786	207.291	187.612	110.204	0.	0.	0.
5700	20.786	207.659	187.960	112.283	0.	0.	0.
5800	20.786	208.021	188.303	114.362	0.	0.	0.
5900	20.786	208.376	188.640	116.440	0.	0.	0.
6000	20.786	208.725	188.972	118.519	0.	0.	0.

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

IP(Ne^+, g) = 330391.0 ± 0.1 cm^{-1}
$S°(298.15\ K)$ = 158.307 ± 0.003 $J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K)$ = 2080.662 ± 0.001 $kJ·mol^{-1}$
$\Delta_f H°(298.15\ K)$ = [2086.966] $kJ·mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^2P_{3/2}$	0	4
$^2P_{1/2}$	780.45	2

Heat of Formation

The ionization limit of neutral neon (173929.70 ± 0.1 cm^{-1}) reported by Moore[1] is adopted as $\Delta_f H°(0\ K)$ for $Ne^+(g)$. 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 ±0.001 $kJ·mol^{-1}$ in the heat of formation. Rosenstock *et al.*[9] and Levin and Lias[11] have summarized additional ionization potential and appearance potential data. 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 0.017 $kJ·mol^{-1}$.

$\Delta_f H°(Ne^+, g, 298.15\ K)$ is obtained from $\Delta_f H°(Ne, g, 0\ K)$ by using IP(Ne) with JANAF[3] enthalpies $H°(0\ K)-H°(298.15\ K)$ for $Ne^+(g)$, Ne(r), and $e^-(r)$. $\Delta_r H°(Ne \rightarrow Ne^+ + e^-, 298.15\ K)$ 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 217000 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 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, 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
	$J·K^{-1}·mol^{-1}$			$kJ·mol^{-1}$			
0	0.	0.	INFINITE	−6.304	2080.662		
100	20.793	135.147	177.401	−4.225			
200	21.262	149.654	160.304	−2.130			
250	21.715	154.447	158.669	−1.056			
298.15	22.119	158.307	158.307	0.	2086.966	2077.139	−363.906
300	22.133	158.444	158.307	0.041	2087.007	2077.078	−361.651
350	22.448	161.881	158.578	1.156	2088.122	2075.336	−309.727
400	22.650	164.893	159.183	2.284	2089.250	2073.432	−270.762
450	22.755	167.567	159.969	3.419	2090.385	2071.387	−240.440
500	22.788	169.967	160.851	4.558	2091.524	2069.215	−216.169
600	22.718	174.118	162.727	6.835	2093.801	2064.539	−179.734
700	22.562	177.609	164.610	9.099	2096.065	2059 483	−153.681
800	22.382	180.610	166.427	11.346	2098.312	2054.103	−134.119
900	22.207	183.236	168.152	13.576	2100.542	2048.443	−118.889
1000	22.048	185.567	169.779	15.788	2102.754	2042.536	−106.691
1100	21.907	187.662	171.311	17.986	2104.952	2036.408	−96.701
1200	21.784	189.562	172.754	20.170	2107.136	2030.080	−88.367
1300	21.678	191.302	174.115	22.343	2109.309	2023.570	−81.308
1400	21.586	192.905	175.400	24.506	2111.472	2016.894	−75.251
1500	21.507	194.391	176.617	26.661	2113.627	2010.063	−69.997
1600	21.438	195.777	177.772	28.808	2115.774	2003.089	−65.394
1700	21.378	197.075	178.870	30.949	2117.915	1995.980	−61.329
1800	21.325	198.295	179.915	33.084	2120.050	1988 746	−57.712
1900	21.279	199.447	180.913	35.214	2122.180	1981.393	−54.472
2000	21.239	200.537	181.868	37.340	2124.306	1973.928	−51.554
2100	21.203	201.573	182.781	39.462	2126.428	1966.357	−48.910
2200	21.171	202.558	183.658	41.580	2128.546	1958.685	−46.505
2300	21.142	203.499	184.501	43.696	2130.662	1950.917	−44.307
2400	21.117	204.398	185.311	45.809	2132.775	1943.057	−42.290
2500	21.094	205.260	186.092	47.919	2134.885	1935.108	−40.432
2600	21.073	206.086	186.845	50.028	2136.994	1927.076	−38.715
2700	21.054	206.881	187.573	52.134	2139.100	1918.962	−37.125
2800	21.037	207.647	188.276	54.239	2141.205	1910.770	−35.646
2900	21.022	208.385	188 957	56.341	2143.307	1902.503	−34.268
3000	21.008	209.097	189.616	58.443	2145.409	1894.164	−32.980
3100	20.995	209.786	190.256	60.543	2147.509	1885.754	−31.775
3200	20.983	210.452	190.877	62.642	2149.608	1877.277	−30.643
3300	20.972	211.098	191.480	64 740	2151.706	1868 734	−29.580
3400	20.962	211.724	192.066	66.836	2153.802	1860.128	−28.577
3500	20.953	212.331	192.636	68.932	2155.898	1851.460	−27.632
3600	20.945	212.921	193.192	71.027	2157.993	1842.732	−26.737
3700	20.937	213.495	193.733	73.121	2160.087	1833.946	−25.891
3800	20.930	214.053	194.260	75.215	2162.181	1825.103	−25.088
3900	20.923	214.597	194.775	77.307	2164.273	1816.206	−24.325
4000	20.916	215.126	195.277	79.399	2166.365	1807.254	−23.600
4100	20.910	215.643	195 767	81.490	2168.456	1798.250	−22.910
4200	20.905	216.147	196.246	83.581	2170.547	1789.196	−22.252
4300	20.900	216 639	196.715	85.671	2172.637	1780.091	−21.624
4400	20.895	217.119	197.173	87.761	2174.727	1770.938	−21.024
4500	20.890	217.589	197.622	89.850	2176.816	1761.737	−20.450
4600	20.886	218.048	198.061	91.939	2178.905	1752.490	−19.900
4700	20.882	218 497	198.491	94 028	2180.994	1743.198	−19.373
4800	20.878	218.936	198.912	96.116	2183.082	1733.861	−18.868
4900	20.875	219.367	199.325	98.203	2185.169	1724.481	−18.383
5000	20.872	219.789	199.730	100.291	2187.257	1715.058	−17.917
5100	20.868	220.202	200.128	102.378	2189.344	1705.593	−17.469
5200	20.865	220.607	200.518	104.464	2191.430	1696 087	−17.037
5300	20.863	221.004	200.900	106.551	2193.517	1686.542	−16.622
5400	20.860	221.394	201.276	108.637	2195.603	1676.957	−16.221
5500	20.857	221.777	201.646	110.723	2197.689	1667.333	−15.835
5600	20.855	222.153	202.009	112.808	2199.774	1657.671	−15.462
5700	20.853	222.522	202.365	114.894	2201.860	1647.972	−15.102
5800	20.850	222.885	202.716	116.979	2203.945	1638.237	−14.754
5900	20.848	223 241	203.061	119.064	2206.030	1628.465	−14.417
6000	20.846	223.591	203.400	121.149	2208.115	1618.658	−14.092

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

REFERENCE STATE

0	to	1728	K	crystal
1728	to	3156.584	K	liquid
above		3156.584	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	−4.786	0.	0.	0.
100	13.631	7.454	50.235	−4.278	0.	0.	0.
200	22.468	20.200	32.143	−2.389	0.	0.	0.
298.15	25.987	29.870	29.870	0.	0.	0.	0.
300	26.024	30.031	29.871	0.048	0.	0.	0.
400	28.493	37.863	30.922	2.776	0.	0.	0.
500	31.045	44.473	32.986	5.743	0.	0.	0.
600	34.853	50.440	35.404	9.022	0.	0.	0.
631.000	39.832	52.263	36.187	10.144	C_p LAMBDA MAXIMUM		
631.000	39.832	52.263	36.187	10.144	TRANSITION		
700	30.794	55.575	37.941	12.344	0.	0.	0.
800	31.003	59.697	40.408	15.431	0.	0.	0.
900	31.589	63.382	42.759	18.560	0.	0.	0.
1000	32.217	66.742	44.992	21.750	0.	0.	0.
1100	32.928	69.845	47.112	25.007	0.	0.	0.
1200	33.681	72.742	49.128	28.336	0.	0.	0.
1300	34.518	75.471	51.051	31.746	0.	0.	0.
1400	35.397	78.061	52.888	35.241	0.	0.	0.
1500	36.317	80.534	54.649	38.827	0.	0.	0.
1600	37.279	82.908	56.342	42.506	0.	0.	0.
1700	38.284	85.199	57.972	46.286	0.	0.	0.
1728.000	38.535	85.827	58.419	47.361	CRYSTAL <--> LIQUID		
1728.000	38.911	95.754	58.419	64.516	TRANSITION		
1800	38.911	97.343	59.944	67.317	0.	0.	0.
1900	38.911	99.446	61.968	71.208	0.	0.	0.
2000	38.911	101.442	63.893	75.099	0.	0.	0.
2100	38.911	103.341	65.726	78.991	0.	0.	0.
2200	38.911	105.151	67.477	82.882	0.	0.	0.
2300	38.911	106.881	69.153	86.773	0.	0.	0.
2400	38.911	108.537	70.760	90.664	0.	0.	0.
2500	38.911	110.125	72.303	94.555	0.	0.	0.
2600	38.911	111.651	73.787	98.446	0.	0.	0.
2700	38.911	113.120	75.217	102.337	0.	0.	0.
2800	38.911	114.535	76.596	106.228	0.	0.	0.
2900	38.911	115.900	77.928	110.120	0.	0.	0.
3000	38.911	117.219	79.216	114.011	0.	0.	0.
3100	38.911	118.495	80.462	117.902	0.	0.	0.
3156.584	38.911	119.199	81.151	120.104	LIQUID <--> IDEAL GAS		
3156.584	22.396	238.807	81.151	497.656	FUGACITY = 1 bar		
3200	22.388	239.113	83.292	498.628	0.	0.	0.
3300	22.373	239.802	88.024	500.866	0.	0.	0.
3400	22.366	240.469	92.498	503.103	0.	0.	0.
3500	22.368	241.118	96.735	505.339	0.	0.	0.
3600	22.377	241.748	100.755	507.576	0.	0.	0.
3700	22.395	242.361	104.573	509.815	0.	0.	0.
3800	22.421	242.959	108.207	512.056	0.	0.	0.
3900	22.456	243.542	111.670	514.299	0.	0.	0.
4000	22.499	244.111	114.974	516.547	0.	0.	0.
4100	22.551	244.667	118.130	518.799	0.	0.	0.
4200	22.611	245.211	121.150	521.058	0.	0.	0.
4300	22.681	245.744	124.041	523.322	0.	0.	0.
4400	22.761	246.266	126.813	525.594	0.	0.	0.
4500	22.850	246.779	129.473	527.875	0.	0.	0.
4600	22.949	247.282	132.029	530.164	0.	0.	0.
4700	23.058	247.777	134.486	532.465	0.	0.	0.
4800	23.178	248.263	136.852	534.776	0.	0.	0.
4900	23.309	248.743	139.130	537.101	0.	0.	0.
5000	23.451	249.215	141.327	539.439	0.	0.	0.
5200	23.769	250.141	145.495	544.160	0.	0.	0.
5400	24.136	251.045	149.387	548.950	0.	0.	0.
5600	24.555	251.930	153.034	553.818	0.	0.	0.
5800	25.028	252.799	156.459	558.775	0.	0.	0.
6000	25.560	253.657	159.685	563.833	0.	0.	0.

PREVIOUS: December 1976 (1 atm) CURRENT: December 1976 (1 bar)