Antoine Coefficients For Vapor Pressure Of the Elements

A comprehensive tabulation for all the important elements from Ac to Zr

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Vapor pressure is important to engineers throughout the chemical process industries (CPI). Knowledge of a compound's vapor pressure is required in the design of storage vessels containing the compound. In hazard analysis, knowledge of vapor pressure is required in the design of the relief valves to protect the system. For design of vapor-liquid operations, such as distillation, knowledge of vapor pressure is required to determine K-values for design and simulation. In environmental applications for liquids in contact with air, knowledge of vapor pressure is required to ascertain concentration in the air and to determine the emissions into the environment.

Results for vapor pressure as a function of temperature are presented here for the chemical elements. The coverage for the elements is comprehensive ranging from Ac to Zr and includes the widely used diatomic elements (Br_2, Cl_2, F_2, H_2, I_2, N_2, and O_2) and inert gases (Ar, He. Ne, and Xe). The results are useable in design, safety, environmental, and simulation applications.

Correlation of vapor pressure

The Antoine equation was selected for correlation of vapor pressure as a function of temperature:

$$\log_{10} P = A - B/(T + C) \quad (1)$$

where P is the vapor pressure (mm Hg); A, B, and C are the Antoine coefficients; and T is the temperature (°C).

The results for vapor pressure are given in Table 1. The tabulation is arranged by alphabetical order (Ac, Al, Am, ..., Zr). This provides ease of use in quickly locating the data by using the chemical formula. The compound name, CAS No (Chemical Abstracts Registry Number), and regression coefficients are provided in the adjacent columns. The range of application is denoted by minimum and maximum temperatures (T_{min} and T_{max}). Temperatures outside the range of application should not be used. The next column provides the code for the tabulation, which is based on both experimental data and estimated values.

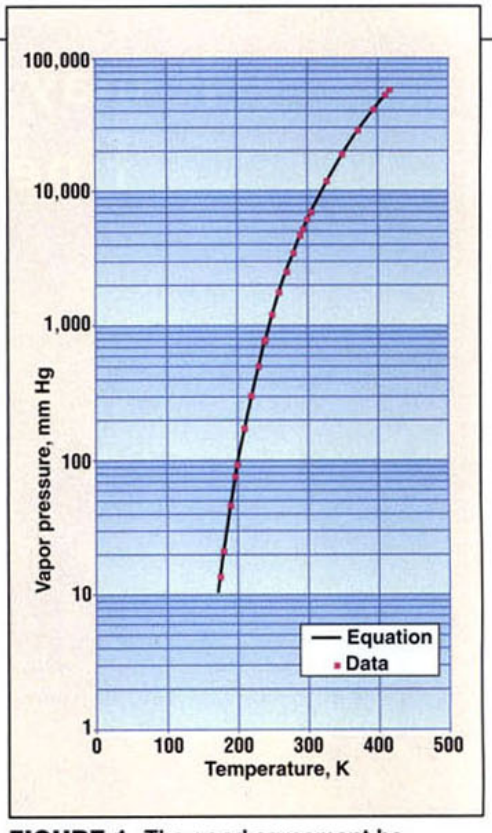

FIGURE 1. The good agreement between the correlation curve and experimental data can be seen in this graph of the vapor pressure of chlorine

In preparing the tabulation, a literature search was conducted to identify data source publications for the elements [*1–17*]. Both experimental values for the physical property under consideration and parameter values for estimation of that property are included in the source publications. The publications were screened and copies

(Continues on p. 54)

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$\log_{10} P = A - B/(T + C)$ (P, mm Hg; T, °C)										
No.	ID	Formula	Name	CAS No	A	B	C	T_{min}	T_{max}	Code
1	1	Ac	actinium	7440-34-8	8.854	2.0735 E+4	273.15	1,599.85	3,198.00	2
2	13	Ag	silver	7440-22-4	8.992	1.5884 E+4	387.39	960.85	6,136.85	1,2
3	77	Al	aluminum	7429-90-5	8.241	1.4525 E+4	192.25	1,209.00	2,517.66	1,2
4	183	Am	americium	7440-35-9	9.188	1.3701 E+4	245.54	726.85	1,126.85	1,2
5	200	Ar	argon	7440-37-1	6.841	3.4027 E+2	271.80	–189.37	–122.29	1,2
6	202	As	arsenic	7440-38-3	9.901	5.8837 E+3	223.24	146.85	614.85	1,2
7	255	At	astatine	7440-68-8	9.515	3.8025 E+3	239.36	5.85	333.85	1,2
8	256	Au	gold	7440-57-5	8.167	1.6053 E+4	180.98	952.85	2,856.00	1,2
9	283	B	boron	7440-42-8	9.375	2.5377 E+4	113.69	1,547.85	3,859.85	1,2
10	416	Ba	barium	7440-39-3	6.477	7.7799 E+3	266.45	638.00	1,897.00	1,2
11	530	Be	beryllium	7440-41-7	8.084	1.3697 E+4	148.52	823.85	2,483.85	1,2
12	562	Bi	bismuth	7440-69-9	7.906	9.0221 E+3	231.44	668.00	1,564.00	1,2
13	633	Br_2	bromine	7726-95-6	7.279	1.3219 E+3	241.80	–7.30	311.00	1,2
14	637	C	carbon (amphorous)	7440-44-0	9.412	2.7489 E+4	281.97	2,985.95	4,125.95	2
14.1	639	C	graphite	7782-42-5	13.639	4.2471 E+4	310.67	2,566.00	3,635.00	1,2
15	675	Ca	calcium	7440-70-2	7.118	7.0844 E+3	188.26	351.85	1,483.85	1,2
16	776	Cd	cadmium	7440-43-9	7.660	4.7576 E+3	228.44	119.85	767.00	1,2
17	830	Ce	cerium	7440-45-1	8.545	2.0813 E+4	231.68	1,719.00	3,443.00	1,2
18	899	Cl_2	chlorine	7782-50-5	7.063	9.0670 E+2	250.83	–101.03	144.00	1,2
19	916	Co	cobalt	7440-48-4	8.775	1.4056 E+4	129.65	821.85	2,254.85	1,2
20	1035	Cr	chromium	7440-47-3	8.487	1.5308 E+4	59.51	1,383.00	2,671.00	1,2
21	1124	Cs	cesium	7440-46-2	6.675	3.5158 E+3	255.57	21.85	671.00	1,2
22	1169	Cu	copper	7440-50-8	8.310	1.5007 E+4	202.14	1,216.00	2,562.00	1,2
23	1302	D_2	deuterium	7782-39-0	6.315	9.2213 E+1	276.35	–254.42	–234.80	1,2
24	1307	Dy	dysprosium	7429-91-6	6.677	9.7586 E+3	3.70	1,105.00	2,567.00	1,2
25	1332	Er	erbium	7440-52-0	7.075	1.2618 E+4	140.57	1,231.00	2,868.00	1,2
26	1369	Eu	europium	7440-53-1	7.354	7.4095 E+3	187.91	366.85	1,468.85	1,2
27	1409	F_2	fluorine	7782-41-4	6.895	3.2010 E+2	267.95	–219.67	–128.84	1,2
28	1420	Fe	iron	7439-89-6	8.379	1.6214 E+4	88.52	1,435.00	2,860.20	1,2
29	1574	Fr	francium	7440-73-5	6.285	3.0994 E+3	237.55	121.00	673.00	2
30	1575	Ga	gallium	7440-55-3	8.285	1.3240 E+4	246.06	680.85	2,204.00	1,2
31	1610	Gd	gadolinium	7440-54-2	8.017	1.7796 E+4	191.64	1,543.00	3,600.00	1,2
32	1637	Ge	germanium	7440-56-4	8.722	1.8108 E+4	273.09	956.85	2,826.85	1,2
33	1709	H_2	hydrogen	1333-74-0	6.149	8.0948 E+1	277.53	–259.20	–239.97	1,2
34	1739	He	helium-4	7440-59-7	5.271	1.3517 E+1	274.58	–271.39	–267.95	1,2
35	1740	Hf	hafnium	7440-58-6	9.065	3.0233 E+4	285.82	1,340.00	4,603.00	1,2
36	1771	Hg	mercury	7439-97-6	7.895	3.1476 E+3	271.10	–38.84	1,461.85	1,2
37	1841	Ho	holmium	7440-60-0	6.662	1.0226 E+4	4.88	1,159.00	2,700.00	1,2
38	1873	I_2	iodine	7553-56-2	7.107	1.5570 E+3	183.97	–31.15	546.00	1,2
39	1877	In	indium	7440-74-6	7.988	1.1857 E+4	249.38	900.00	2,072.00	1,2
40	1917	Ir	iridium	7439-88-5	9.227	2.8611 E+4	80.35	2,200.00	4,428.00	1,2
41	1960	K	potassium	7440-09-7	6.974	4.1439 E+3	254.47	63.20	1,949.85	1,2
42	2162	Kr	krypton	7439-90-9	7.014	5.1162 E+2	277.13	– 157.37	–63.80	1,2
43	2168	La	lanthanum	7439-91-0	8.578	2.1097 E+4	239.17	1,650.00	3,464.00	1,2
44	2203	Li	lithium	7439-93-2	8.269	8.8846 E+3	307.17	180.54	3,811.85	1,2
45	2316	Lu	lutetium	7439-94-3	7.832	1.7422 E+4	116.75	1,600.00	3,402.00	1,2
46	2335	Mg	magnesium	7439-95-4	7.706	6.3030 E+3	216.22	243.85	1,090.00	1,2
47	2464	Mn	manganese	7439-96-5	7.796	1.0766 E+4	129.43	650.85	2,061.00	1,2
48	2548	Mo	molybdenum	7439-98-7	8.649	2.6943 E+4	31.68	2,400.00	4,950.00	1,2
49	2678	N_2	nitrogen	7727-37-9	6.725	2.8557 E+2	270.09	–210.00	–147.05	1,2
50	2781	Na	sodium	7440-23-5	7.488	5.3001 E+3	267.61	97.82	2,299.85	1,2
51	3019	Nb	niobium	7440-03-1	9.943	3.5065 E+4	221.05	1,976.85	4,744.00	1,2
52	3057	Nd	neodymium	7440-00-8	7.369	1.4888 E+4	243.34	870.85	3,074.00	1,2
53	3091	Ne	neon	7440-01-9	6.744	1.1533 E+2	275.91	–248.59	–228.75	1,2
54	3092	Ni	nickel	7440-02-0	8.764	1.7954 E+4	138.85	1,480.00	3,200.00	1,2
55	3182	Np	neptunium	7439-99-8	7.032	1.9215 E+4	158.97	1,344.84	1,800.84	2
56	3198	O_2	oxygen	7782-44-7	6.837	3.3921 E+2	268.70	–218.80	–118.57	1,2
57	3200	Os	osmium	7440-04-2	9.765	3.4751 E+4	35.61	2,600.00	5,400.00	1,2
58	3234	P	phosphorus (white)	7723-14-0	7.063	2.0166 E+3	201.67	131.00	317.00	1,2

code: 1 - data, 2 - estimate

(Continues on p. 54)

(Continued from p. 53) $\log_{10} P = A - B/(T + C)$ (P, mm Hg; T, °C)

No.	ID	Formula	Name	CAS No	A	B	C	T_{min}	T_{max}	Code
58.1	3235	P	phosphorus (red)	7723-14-0	8.183	2.7187 E+3	81.75	182.00	720.85	1,2
59	3483	Pb	lead	7439-92-1	7.463	9.1318 E+3	243.70	434.85	1,749.00	1,2
60	3571	Pd	palladium	7440-05-3	8.568	1.8403 E+4	273.14	1,300.00	3,400.00	1,2
61	3641	Po	polonium	7440-08-6	7.184	5.2650 E+3	261.55	500.00	1,050.00	1,2
62	3650	Pr	praseodymium	7440-10-0	6.781	1.4031 E+4	77.80	1,497.70	3,520.00	1,2
63	3691	Pt	platinum	7440-06-4	8.586	2.2056 E+4	41.02	1,470.85	3,825.00	1,2
64	3756	Pu	plutonium	7440-07-5	8.087	1.8532 E+4	331.78	1,483.00	3,228.00	1,2
65	3773	Ra	radium	7440-14-4	6.716	6.6225 E+3	200.78	319.85	1,526.00	1,2
66	3781	Rb	rubidium	7440-17-7	7.000	3.9262 E+3	265.16	36.85	688.00	1,2
67	3828	Re	rhenium	7440-15-5	8.976	3.4838 E+4	119.34	2,206.85	5,596.00	1,2
68	3880	Rh	rhodium	7440-16-6	9.685	2.6834 E+4	248.59	1,461.85	3,695.00	1,2
69	3940	Rn	radon	10043-92-2	6.580	6.5167 E+2	237.86	–160.00	103.85	1,2
70	3941	Ru	ruthenium	7440-18-8	9.286	2.6794 E+4	33.09	2,200.00	4,500.00	1,2
71	3991	S	sulfur	7704-34-9	7.866	3.4650 E+3	250.34	115.21	1,039.85	1,2
72	4023	Sb	antimony	7440-36-0	5.881	4.9847 E+3	74.32	343.85	1,587.00	1,2
73	4065	Sc	scandium	7440-20-2	7.726	1.3961 E+4	45.18	1,300.00	3,200.00	1,2
74	4083	Se	selenium (gray)	7782-49-2	7.054	3.4420 E+3	139.77	123.85	685.00	1,2
75	4140	Si	silicon	7440-21-3	9.326	2.3320 E+4	401.58	1,500.00	3,400.00	1,2
76	4303	Sm	samarium	7440-19-9	6.724	7.2428 E+3	90.48	700.00	2,000.00	1,2
77	4332	Sn	tin (white)	7440-31-5	8.549	1.6656 E+4	336.40	1,150.00	2,800.00	1,2
78	4461	Sr	strontium	7440-24-6	6.832	6.1287 E+3	168.97	308.85	1,382.00	1,2
79	4517	Ta	tantalum	7440-25-7	8.733	3.1264 E+4	–115.81	2,237.85	5,458.00	1,2
80	4550	Tb	terbium	7440-27-9	7.418	1.4825 E+4	37.37	1,516.10	3,230.00	1,2
81	4570	Tc	technetium	7440-26-8	26.085	2.3683 E+5	5941.04	2,400.00	4,400.00	1,2
82	4583	Te	tellurium	13494-80-9	6.639	4.0844 E+3	98.94	223.85	988.00	1,2
83	4609	Th	thorium	7440-29-1	8.087	2.5785 E+4	165.09	2360.00	4788.00	1,2
84	4639	Ti	titanium	7440-32-6	10.736	2.8593 E+4	473.29	1234.85	3168.85	1,2
85	4703	Tl	thallium	7440-28-0	7.615	8.0601 E+3	229.50	362.85	1473.00	1,2
86	4747	Tm	thulium	7440-30-4	8.210	1.0716 E+4	200.67	387.85	963.85	1,2
87	4766	U	uranium	7440-61-1	8.273	2.3313 E+4	190.15	2000.00	4200.00	1,2
88	4836	V	vanadium	7440-62-2	9.228	2.2303 E+4	133.69	1330.85	3380.00	1,2
89	4899	W	tungsten	7440-33-7	9.983	4.0388 E+4	131.64	3204.00	5555.00	1,2
90	4945	Xe	xenon	7440-63-3	6.673	5.4580 E+2	252.04	-190.00	16.59	1,2
91	4960	Y	yttrium	7440-65-5	8.005	1.7992 E+4	165.95	1610.10	3345.00	1,2
92	4995	Yb	ytterbium	7440-64-4	7.281	6.0602 E+3	181.30	463.00	1196.00	1,2
93	5021	Zn	zinc	7440-66-6	8.447	6.8192 E+3	318.01	419.55	2896.85	1,2
94	5113	Zr	zirconium	7440-67-7	9.122	2.8774 E+4	201.25	1701.85	4409.00	1,2

code: 1 - data, 2 - estimate

of appropriate data were made. These data were then keyed into the computer thereby providing a database of values for compounds for which experimental data are available. The database also served as a basis to check the accuracy of the estimation methods. Upon completion of data collection, estimation of the values for the remaining compounds was performed. The numerous point values were processed using a computer program for minimum deviation.

The compilations of CRC [*1*], Daubert and Danner [*2*], Hultgren [*3*], TAMU [*7, 8*], and Yaws [*11–17*] were used extensively for identification of data sources. Estimates were primarily based on literature estimated values and proprietary techniques developed by the author.

A comparison of calculated and data values is shown in Figure 1 for a representative compound. The graph discloses favorable agreement of equation and data.

An example

To illustrate how to use Table 1, an example is presented. Suppose you are interested in finding the vapor pressure of chlorine (Cl_2) at 26.81°C. To calculate the vapor pressure, simply substitute the Antoine coefficients for Cl_2 from Table 1 and the temperature into Equation 1. This yields:

$\log_{10} P = 7.06306 - 906.7031/(26.81 + 250.83) = 3.7973$

$P = 10^{3.7973} = 6{,}270$ mm Hg ■

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