VAN DER WAALS CONSTANTS FOR GASES

The van der Waals equation of state for a real gas is

$$(P + n^2a/V^2)(V - nb) = nRT$$

where P is the pressure, V the volume, T the temperature, n the amount of substance (in moles), and R the gas constant. The van der Waals constants a and b are characteristic of the substance and are independent of temperature. They are related to the critical temperature and pressure, T_c and P_c , by

$$a = 27R^2T_{\rm c}^2/64P_{\rm c}$$
 $b = RT_{\rm c}/8P_{\rm c}$

This table gives values of a and b for some common gases. Most of the values have been calculated from the critical temperature and pressure values given in the table "Critical Constants" in this section. Van der Waals constants for other gases may easily be calculated from the data in that table

To convert the van der Waals constants to SI units, note that 1 bar L²/mol² = 0.1 Pa m⁶/mol² and 1 L/mol = 0.001 m³/mol.

REFERENCE

Reid, R.C., Prausnitz, J. M., and Poling, B.E., The Properties of Gases and Liquids, Fourth Edition, McGraw-Hill, New York, 1987.

	a	b		a	b
Substance	$bar\ L^2\!/mol^2$	L/mol	Substance	$bar\ L^2/mol^2$	L/mol
Acetic acid	17.71	0.1065	Hydrogen sulfide	4.544	0.0434
Acetone	16.02	0.1124	Isobutane	13.32	0.1164
Acetylene	4.516	0.0522	Krypton	5.193	0.0106
Ammonia	4.225	0.0371	Methane	2.303	0.0431
Aniline	29.14	0.1486	Methanol	9.476	0.0659
Argon	1.355	0.0320	Methylamine	7.106	0.0588
Benzene	18.82	0.1193	Neon	0.208	0.0167
Bromine	9.75	0.0591	Neopentane	17.17	0.1411
Butane	13.89	0.1164	Nitric oxide	1.46	0.0289
1-Butanol	20.94	0.1326	Nitrogen	1.370	0.0387
2-Butanone	19.97	0.1326	Nitrogen dioxide	5.36	0.0443
Carbon dioxide	3.658	0.0429	Nitrogen trifluoride	3.58	0.0545
Carbon disulfide	11.25	0.0726	Nitrous oxide	3.852	0.0444
Carbon monoxide	1.472	0.0395	Octane	37.88	0.2374
Chlorine	6.343	0.0542	1-Octanol	44.71	0.2442
Chlorobenzene	25.80	0.1454	Oxygen	1.382	0.0319
Chloroethane	11.66	0.0903	Ozone	3.570	0.0487
Chloromethane	7.566	0.0648	Pentane	19.09	0.1449
Cyclohexane	21.92	0.1411	1-Pentanol	25.88	0.1568
Cyclopropane	8.34	0.0747	Phenol	22.93	0.1177
Decane	52.74	0.3043	Propane	9.39	0.0905
1-Decanol	59.51	0.3086	1-Propanol	16.26	0.1079
Diethyl ether	17.46	0.1333	2-Propanol	15.82	0.1109
Dimethyl ether	8.690	0.0774	Propene	8.442	0.0824
Dodecane	69.38	0.3758	Pyridine	19.77	0.1137
1-Dodecanol	75.70	0.3750	Pyrrole	18.82	0.1049
Ethane	5.580	0.0651	Silane	4.38	0.0579
Ethanol	12.56	0.0871	Sulfur dioxide	6.865	0.0568
Ethylene	4.612	0.0582	Sulfur hexafluoride	7.857	0.0879
Fluorine	1.171	0.0290	Tetrachloromethane	20.01	0.1281
Furan	12.74	0.0926	Tetrachlorosilane	20.96	0.1470
Helium	0.0346	0.0238	Tetrafluoroethylene	6.954	0.0809
Heptane	31.06	0.2049	Tetrafluoromethane	4.040	0.0633
1-Heptanol	38.17	0.2150	Tetrafluorosilane	5.259	0.0724
Hexane	24.84	0.1744	Tetrahydrofuran	16.39	0.1082
1-Hexanol	31.79	0.1856	Thiophene	17.21	0.1058
Hydrazine	8.46	0.0462	Toluene	24.86	0.1497
Hydrogen	0.2452	0.0265	1,1,1-Trichloroethane	20.15	0.1317
Hydrogen bromide	4.500	0.0442	Trichloromethane	15.34	0.1019
Hydrogen chloride	3.700	0.0406	Trifluoromethane	5.378	0.0640
Hydrogen cyanide	11.29	0.0881	Trimethylamine	13.37	0.1101
Hydrogen fluoride	9.565	0.0739	Water	5.537	0.0305
Hydrogen iodide	6.309	0.0530	Xenon	4.192	0.0516
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