

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

$$\left[P + a \left(\frac{n}{V} \right)^2 \right] (V - n \cdot b) = nRT$$

where P is the pressure, V the volume, T the absolute temperature, n the amount of substance in moles, and R the gas constant. The constants a and b have positive values and are characteristic of the individual gas.

To convert 'a' into atm L²/mol² multiply by 0.98692 atm/bar

To convert 'a' into kPa L²/mol² multiply by 100.0 kPa/bar

Gas	a bar·L ² /mol ²	b L/mol	Gas	a bar·L ² /mol ²	b L/mol
Acetic acid	17.82	0.1068	Dodecane	69.38	0.3758
Acetic anhydride	20.16	0.1263	1-Dodecanol	75.70	0.3750
Acetone	14.09	0.0994	Ethane	5.562	0.0638
Acetonitrile	17.81	0.1168	Ethanethiol	11.39	0.08098
Acetylene	4.448	0.05136	Ethanol	12.18	0.08407
Aluminium trichloride	42.63	0.2450	Ethyl acetate	20.72	0.1412
Ammonium chloride	2.380	0.00734	Ethylamine	10.74	0.08409
Ammonia	4.225	0.03713	Ethylene	4.612	0.0582
Aniline	29.14	0.1486	Fluorine	1.171	0.02896
Argon	1.363	0.03219	Fluorobenzene	20.19	0.1286
Benzene	18.24	0.1154	Fluoromethane	4.692	0.05264
Boron trichloride	15.60	0.1222	Freon	10.78	0.0998
Boron trifluoride	3.98	0.05443	Furan	12.74	0.0926
Bromine	9.75	0.0591	Germane	5.743	0.06555
Bromobenzene	28.94	0.1539	Germanium tetrachloride	22.90	0.1485
Butane	14.66	0.1226	Helium	0.03457	0.0237
1-Butanol	20.94	0.1326	Heptane	31.06	0.2049
Butanone	19.97	0.1326	1-Heptanol	38.17	0.2150
Carbon dioxide	3.640	0.04267	Hexane	24.71	0.1735
Carbon disulfide	11.77	0.07685	1-Hexanol	31.79	0.1856
Carbon monoxide	1.505	0.03985	Hydrazine	8.46	0.0462
Carbon tetrachloride	19.7483	0.1281	Hydrogen	0.2452	0.02661
Chlorine	6.579	0.05622	Hydrogen bromide	4.510	0.04431
Chlorine pentafluoride	9.58	0.08204	Hydrogen chloride	3.716	0.04081
Chlorobenzene	25.77	0.1453	Hydrogen cyanide	11.29	0.0881
Chloroethane	11.05	0.08651	Hydrogen fluoride	9.565	0.0739
Chloromethane	7.570	0.06483	Hydrogen iodide	6.309	0.0530
Cyanogen	7.769	0.06901	Hydrogen selenide	5.338	0.04637
Cyclohexane	23.11	0.1424	Hydrogen sulfide	4.490	0.04287
Cyclopropane	8.34	0.0747	Iodobenzene	33.52	0.1656
Decane	52.74	0.3043	Isobutane	13.32	0.1164
1-Decanol	59.51	0.3086	Krypton	2.349	0.03978
Diborane	6.048	0.07437	Mercury	5.193	0.01057
Diethyl ether	17.46	0.1333	Methane	2.283	0.04278
Diethyl sulfide	19.00	0.1214	Methanol	9.649	0.06702
Dimethyl ether	8.180	0.07246	Methylamine	7.106	0.0588
Dimethyl sulfide	13.04	0.09213	Neon	0.2135	0.01709

Gas	a bar-L ² /mol ²	b L/mol	Gas	a bar-L ² /mol ²	b L/mol
Neopentane	17.17	0.1411	Radon	6.601	0.06239
Nitric oxide	1.358	0.02789	Silane	4.38	0.0579
Nitrogen	1.408	0.03913	Silicon tetrachloride	20.96	0.1470
Nitrogen dioxide	5.354	0.04424	Silicon tetrafluoride	4.251	0.05571
Nitrogen trifluoride	3.58	0.05453	Sulfur dioxide	6.865	0.0568
Nitrous oxide	3.852	0.04435	Sulfur hexafluoride	7.857	0.0879
Octane	37.88	0.2374	Tetrachloromethane	20.01	0.1281
1-Octanol	44.71	0.2442	Tetrachlorosilane	20.96	0.1470
Oxygen	1.378	0.03183	Tetrafluoroethylene	6.954	0.0809
Ozone	3.570	0.0487	Tetrafluorohydrazine	7.426	0.08564
Pentane	19.26	0.1449	Tetrafluoromethane	4.040	0.0633
1-Pentanol	25.88	0.1568	Tetrafluorosilane	5.259	0.0724
Phenol	22.93	0.1177	Tetrahydrofuran	16.39	0.1082
Phosphine	4.692	0.05156	Thiophene	17.21	0.1058
Phosphonium chloride	4.111	0.04545	Tin tetrachloride	27.27	0.1642
Phosphorus	53.6	0.157	Titanium(IV) chloride	25.47	0.1423
Phosphorus trifluoride	4.954	0.06510	Toluene	24.38	0.1463
Propane	9.39	0.0905	1,1,1-Trichloroethane	20.15	0.1317
1-Propanol	16.26	0.1079	Trichloromethane	15.34	0.1019
2-Propanol	15.82	0.1109	Trifluoromethane	5.378	0.0640
Propene	8.442	0.0824	Trimethylamine	13.37	0.1101
Pyridine	19.77	0.1137	Water vapor	5.536	0.03049
Pyrrole	18.82	0.1049	Xenon	4.250	0.05105

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