van der Waal's Constants for Real Gases

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

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

To convert '*a*' into atm L^2/mol^2 multiply by 0.986 atm/bar
To convert '*a*' into kPa L^2/mol^2 multiply by 100.0 kPa/bar

Molecular Formula	Name	*a* bar L^2/mol^2	*b* L/mol
$AlCl_3$	Aluminum trichloride	42.63	0.2450
NH_3	Ammonia	4.225	0.03713
NH_4Cl	Ammonium chloride	2.380	0.00734
Ar	Argon	1.355	0.03201
BCl_3	Boron trichloride	15.60	0.1222
BF_3	Boron trifluoride	3.98	0.05443
B_2H_6	Diborane	6.048	0.07437
Br_2	Bromine	9.75	0.0591
$ClFO_2$	Perchloryl fluoride	7.371	0.07130
ClF_5	Chlorine pentafluoride	9.58	0.08204
ClH_4P	Phosphonium chloride	4.111	0.04545
Cl_2	Chlorine	6.343	0.05422
Cl_3FSi	Trichlorofluorosilane	15.67	0.1273
F_2	Fluorine	1.171	0.02896
$GeCl_4$	Germanium tetrachloride	23.12	0.1489
F_3N	Nitrogen trifluoride	3.58	0.05453
F_3P	Phosphorus trifluoride	4.954	0.06510
F_4N_2	Tetrafluorohydrazine	7.426	0.08564
GeH_4	Germane	5.743	0.06555
He	Helium	0.0346	0.0238
HBr	Hydrogen bromide	4.500	0.04415
HCl	Hydrogen chloride	3.700	0.04061
HCN	Hydrogen cyanide	11.29	0.08806
HF	Hydrogen fluoride	9.565	0.0739
HI	Hydrogen iodide	6.309	0.05303
H_2	Hydrogen	0.2453	0.02651
H_2O	Water	5.537	0.03049
H_2S	Hydrogen sulphide	4.544	0.04339
H_2Se	Hydrogen selenide	5.523	0.0479
Kr	Krypton	2.325	0.0396
SiH_4	Silane	4.38	0.0579
$SiCl_4$	Silicon tetrachloride	20.96	0.1470
SiF_4	Silicon tetrafluoride	5.259	0.07236
$TiCl_4$	Titanium(IV) chloride	25.47	0.1423
Hg	Mercury	5.193	0.01057
NO	Nitric oxide	1.46	0.0289
NO_2	Nitrogen dioxide	5.36	0.0443
N_2	Nitrogen	1.370	0.0387
N_2O	Nitrous oxide	3.852	0.04435
N_2H_4	Hydrazine	8.46	0.0462
Ne	Neon	0.208	0.01672
O_2	Oxygen	1.382	0.03186
O_3	Ozone	3.570	0.0487
P	Phosphorus	53.6	0.157
PH_3	Phosphine	4.696	0.05157
Rn	Radon	6.601	0.06239
$SnCl_4$	Stannic chloride	27.25	0.1641
S	Sulphur	24.3	0.0660

SO_2	Sulphur dioxide	6.865	0.05679
SF_6	Sulphur hexafluoride	7.857	0.08786
Se	Selenium	33.4	0.0675
UF_6	Uranium(VI) fluoride	16.01	0.1128
WF_6	Tungsten(VI) fluoride	13.25	0.1063
Xe	Xenon	4.192	0.05156
XeF_2	Xenon difluoride	12.46	0.07037
XeF_4	Xenon tetrafluoride	15.52	0.09035
$CClF_3$	Chlorotrifluoromethane	6.873	0.08110
CCl_3F	Trichlorofluoromethane	14.68	0.1111
CCl_4	Tetrachloromethane	20.01	0.1281
CF_4	Tetrafluoromethane	4.040	0.06325
CO	Carbon monoxide	1.472	0.03948
COS	Carbon oxysulphide	6.975	0.06628
CO_2	Carbon dioxide	3.658	0.04286
CS_2	Carbon disulphide	11.25	0.07262
$CHCl_3$	Trichloromethane	15.34	0.1019
CHF_3	Trifluoromethane	5.378	0.06403
CH_2Cl_2	Dichloromethane	12.44	0.08689
CH_2F_2	Difluoromethane	6.184	0.06268
CH_3Cl	Chloromethane	7.566	0.06477
CH_3F	Fluoromethane	5.009	0.05617
NH_3NO_2	Nitromethane	17.18	0.1041
CH_4	Methane	2.300	0.04301
CH_3OH	Methanol	9.472	0.06584
CH_3SH	Methanethiol	8.911	0.06756
CH_3NH_2	Methylamine	7.106	0.05879
$C_2Cl_2F_3$	1,1,2-Trichlorotrifluoroethane	20.25	0.1481
C_2F_4	Tetrafluoroethylene	6.954	0.08085
C_2N_2	Cyanogen	7.803	0.6952
C_2H_2	Acetylene	4.516	0.05220
$C_2H_2F_2$	1,1-Difluoroethylene	6.000	0.07058
$C_2H_3Cl_3$	1,1,1-Trichloroethane	20.15	0.1317
C_2H_3F	Fluroethylene	5.984	0.06504
$C_2H_3F_3$	1,1,1-Trifluoroethane	9.302	0.09572
C_2H_3N	Acetonitrile	17.89	0.1169
C_2H_4	Ethylene	4.612	0.05821
$C_2H_4Cl_2$	1,1-Dichloroethane	15.73	0.1072
$C_2H_4Cl_2$	1,2-Dichloroethane	17.0	0.108
C_2H_4O	Ethylene oxide	8.922	0.06779
CH_3COOH	Acetic acid	17.71	0.1065
$C_2H_4O_2$	Methyl formate	11.54	0.08442
C_2H_5Br	Bromoethane	11.89	0.08406
C_2H_5Cl	Chloroethane	11.7	0.090
C_2H_5F	Fluoroethane	8.170	0.07758
C_2H_6	Ethane	5.570	0.06499
C_2H_6O	Dimethyl ether	8.690	0.07742
C_2H_5OH	Ethanol	12.56	0.08710
C_2H_5SH	Dimethyl sulphide	13.34	0.09453
C_2H_5SH	Ethanethiol	13.23	0.09447
C_2H_7N	Dimethylamine	10.44	0.08510
C_2H_7N	Ethylamine	10.79	0.08433
C_3F_8	Perfluoropropane	12.96	0.1338

C_3H_5N	Propanenitrile	21.57	0.1369
C_3H_6	Propene	8.438	0.08242
C_3H_6	Cyclopropane	8.293	0.07420
C_3H_6O	Acetone	16.02	0.1124
C_3H_6O	Propanal	14.08	0.09947
$C_3H_6O_2$	Ethyl formate	15.91	0.1115
$C_3H_6O_2$	Methyl acetate	15.75	0.1108
$C_3H_6O_2$	Propanoic acid	23.49	0.1386
C_3H_7Cl	1-Chloropropane	16.11	0.1141`
C_3H_8	Propane	9.385	0.09044
C_3H_8O	1-Propanol	16.26	0.1080
C_3H_8O	2-Propanol	15.82	0.1109
C_3H_8O	Ethyl methyl ether	12.70	0.1034
C_3H_8S	Ethyl methyl sulphide	19.45	0.1300
C_3H_9N	Propylamine	15.26	0.1094
C_3H_9N	Trimethylamine	13.37	0.1101
C_4H_4O	Furan	12.74	0.0926
C_4H_4S	Thiophene	17.21	0.1058
C_4H_4N	Pyrrole	18.82	0.1049
C_4H_6	1,3-Butadiene	12.17	0.1020
$C_4H_6O_3$	Acetic anhydride	26.8	0.157
C_4H_7N	Butanenitrile	25.76	0.1568
C_4H_8	1-Butene	12.76	0.1084
C_4H_8	Cyclobutane	12.39	0.0960
C_4H_8O	2-Butanone	19.97	0.1326
C_4H_8O	Tetrahydrofuran	16.39	0.1082
$C_4H_8O_2$	1,4-Dioxane	19.29	0.1171
$C_4H_8O_2$	Ethyl acetate	20.57	0.1401
$C_4H_8O_2$	Methyl propanoate	20.51	0.1377
$C_4H_8O_2$	Propyl formate	20.79	0.1377
$C_4H_8O_2$	Butanoic acid	28.18	0.1609
C_4H_9N	Pyrrolidine	16.84	0.1056
C_4H_{10}	Butane	13.93	0.1168
C_4H_{10}	Isobutane	13.36	0.1168
$C_4H_{10}O$	1-Butanol	20.90	0.1323
$C_4H_{10}O$	2-Methyl-2-propanol	18.81	0.1324
$C_4H_{10}O$	2-Methyl-1-propanol	20.35	0.1324
$C_4H_{10}O$	Diethyl ether	17.46	0.1333
$C_4H_{10}S$	Diethyl sulphide	22.85	0.1462
$C_4H_{11}N$	Butylamine	19.41	0.1301
$C_4H_{11}N$	Diethylamine	19.40	0.1383
$C_4H_{12}Si$	Tetramethylsilane	20.81	0.1653
$C_5H_4O_2$	Furfural	22.23	0.1182
C_5H_5N	Pyridine	19.77	0.1137
C_5H_8	Cyclopentene	15.61	0.1097
C_5H_{10}	1-Pentene	17.86	0.1370
C_5H_{10}	2-Methyl-1-butene	16.9	0.129
C_5H_{10}	2-Methyl-2-butene	17.26	0.1279
C_5H_{10}	Cyclopentane	16.94	0.1180
$C_5H_{10}O$	Tetrahydropyran	20.02	0.1247
$C_5H_{10}O_2$	Isobutyl formate	22.82	0.1476
$C_5H_{10}O_2$	Propyl acetate	26.23	0.1700

$C_5H_{10}O_2$	**Ethyl propanoate**	**25.86**	**0.1688**
$C_5H_{10}O_2$	**Methyl butanoate**	**25.83**	**0.1661**
$C_5H_{10}O_2$	**Methyl isobutanoate**	**24.87**	**0.1639**
$C_5H_{11}N$	**Piperidine**	**20.84**	**0.1250**
C_5H_{12}	**Pentane**	**19.13**	**0.1451**
C_5H_{12}	**Isopentane**	**18.29**	**0.1415**
C_5H_{12}	**Neopentane**	**17.17**	**0.1410**
$C_5H_{12}O$	**1-Pentanol**	**25.81**	**0.1564**
C_6H_5Br	**Bromobenzene**	**28.96**	**0.1541**
C_6H_5Cl	**Chlorobenzene**	**25.80**	**0.1454**
C_6H_5F	**Fluorobenzene**	**20.10**	**0.1279**
C_6H_5I	**Iodobenzene**	**33.54**	**0.1658**
C_6H_6	**Benzene**	**18.82**	**0.1193**
C_6H_5OH	**Phenol**	**22.93**	**0.1177**
$C_6H_5NH_2$	**Aniline**	**29.14**	**0.1486**
$C_6H_{10}O$	**Cyclohexanone**	**31.1**	**0.170**
$C_6H_{11}N$	**Hexanenitrile**	**35.50**	**0.1996**
C_6H_{12}	**Cyclohexane**	**21.95**	**0.1413**
$C_6H_{11}OH$	**Cyclohexanol**	**28.93**	**0.1586**
$C_6H_{12}O_2$	**Pentyl formate**	**27.97**	**0.1730**
$C_6H_{12}O_2$	**Isobutyl acetate**	**29.05**	**0.1845**
$C_6H_{12}O_2$	**Ethyl butanoate**	**30.53**	**0.1922**
$C_6H_{12}O_2$	**Ethyl 2-methylpropanoate**	**29.05**	**0.1872**
$C_6H_{12}O_2$	**Methyl pentanoate**	**29.39**	**0.1847**
C_6H_{14}	**Hexane**	**24.97**	**0.1753**
C_6H_{14}	**2,3-Dimethylbutane**	**23.29**	**0.1660**
$C_6H_{14}O$	**1-Hexanol**	**31.35**	**0.1829**
$C_6H_{15}N$	**Triethylamine**	**27.59**	**0.1836**
$C_6H_{15}N$	**Dipropylamine**	**24.82**	**0.1591**
C_7H_5N	**Benzonitrile**	**33.89**	**0.1727**
C_7H_6O	**Benzaldehyde**	**30.30**	**0.1553**
C_7H_8	**Toluene**	**24.89**	**0.1499**
C_7H_8O	***o*-Cresol**	**28.33**	**0.1447**
C_7H_8O	***m*-Cresol**	**31.86**	**0.1609**
C_7H_8O	***p*-Cresol**	**28.11**	**0.1422**
C_7H_8O	**Benzyl alcohol**	**34.7**	**0.173**
C_7H_8O	**Anisole**	**28.60**	**0.1579**
C_7H_{16}	**Heptane**	**30.89**	**0.2038**
$C_7H_{15}OH$	**Heptanol**	**37.22**	**0.2097**
C_8H_{10}	**Ethylbenzene**	**30.86**	**0.1782**
C_8H_{10}	***o*-Xylene**	**31.06**	**0.1756**
C_8H_{10}	***m*-Xylene**	**31.41**	**0.1814**
C_8H_{10}	***p*-Xylene**	**31.54**	**0.1824**
$C_8H_{10}O$	**Phenetole**	**35.70**	**0.1966**
$C_8H_{11}N$	**N,N-Dimethylaniline**	**37.92**	**0.1967**
C_8H_{18}	**Octane**	**37.86**	**0.2372**
C_8H_{18}	**2,5-Dimethylhexane**	**35.49**	**0.2299**
$C_8H_{18}O$	**1-Octanol**	**43.42**	**0.2371**
C_9H_7N	**Quinoline**	**36.70**	**0.1672**
C_9H_{12}	**Cumene**	**36.20**	**0.2044**
C_9H_{12}	**Propylbenzene**	**37.14**	**0.2073**
C_9H_{12}	**1,2,4-Trimethylbenzene**	**38.03**	**0.2088**

C_9H_{12}	**Mesitylene**	**37.87**	**0.2118**
C_9H_{20}	**Nonane**	**45.11**	**0.2702**
$C_9H_{20}O$	**1-Nonanol**	**50.00**	**0.2654**
$C_{10}H_8$	**Naphthalene**	**40.32**	**0.1920**
$C_{10}H_{14}$	**Butylbenzene**	**44.07**	**0.2378**
$C_{10}H_{14}$	**Isobutylbenzene**	**40.40**	**0.2215**
$C_{10}H_{14}$	***o*-Cymene**	**42.7**	**0.234**
$C_{10}H_{14}$	***p*-Cymene**	**45.27**	**0.2478**
$C_{10}H_{14}$	**p-Diethylbenzene**	**45.03**	**0.2439**
$C_{10}H_{14}$	**1,2,4,5-Tetramethylbenzene**	**45.8**	**0.24**
$C_{10}H_{22}$	**Decane**	**52.88**	**0.3051**
$C_{10}H_{22}O$	**1-Decanol**	**57.45**	**0.2971**
$C_{11}H_{24}$	**Undecane**	**60.88**	**0.3396**
$C_{12}H_{10}$	**Biphenyl**	**47.16**	**0.2130**
$C_{12}H_{26}$	**Dodecane**	**69.14**	**0.3741**
$C_{12}H_{26}O$	**1-Dodecanol**	**72.69**	**0.3598**
$C_{13}H_{12}$	**Diphenylmethane**	**60.46**	**0.2798**
$C_{13}H_{28}$	**Tridecane**	**77.94**	**0.4109**
$C_{13}H_{28}O$	**1-Tridecanol**	**81.20**	**0.3942**
$C_{14}H_{30}O$	**1-Tetradecanol**	**89.91**	**0.4289**
$C_{15}H_{32}$	**Pentadecane**	**96.50**	**0.4857**