

Molecule name	logK _{aw} exp	logK _{aw} calc	Deviation
1,1,3-Trimethylcyclopentane	1.81	0.97	0.84
1,3,5-Cycloheptatriene	-0.74	-0.97	0.23
1,4-Cyclohexadiene	-0.51	-0.81	0.30
1,4-Pentadiene	0.68	0.21	0.47
1,5-Hexadiene	0.74	0.27	0.47
1,6-Heptadiene	0.86	0.38	0.48
1,6-Heptadiyne	-1.06	-0.88	-0.18
1,8-Nonadiyne	-0.87	-0.76	-0.11
1-Butene	0.98	0.16	0.82
1-Butyne	-0.14	-0.47	0.33
1-Decene	1.60	0.55	1.05
1-Heptene	1.22	0.34	0.88
1-Heptyne	0.44	-0.26	0.70
1-Hexene	1.16	0.28	0.88
1-Hexyne	0.19	-0.35	0.54
1-Methyl-4-isopropylcyclohexene	-0.07	-0.17	0.10
1-Methylcyclohexene	0.49	-0.56	1.05
1-Nonene	1.51	0.46	1.05
1-Nonyne	0.77	-0.14	0.91
1-Octyne	0.52	-0.20	0.72
1-Pentadecene	2.25	0.85	1.40
1-Pentene	1.22	0.25	0.97
1-Pentyne	-0.12	-0.41	0.29
1-trans-5-trans-9-cis-Cyclododecatriene	0.36	-0.68	1.04
2,2,3,3-Tetramethylbutane	1.99	2.08	-0.09
2,2,3-Trimethylhexane	2.34	1.90	0.44
2,2,3-Trimethylpentane	1.92	1.75	0.17
2,2,5,5-Tetramethyl-3-hexyne	1.08	0.51	0.57
2,2,5-Trimethyl-3-hexyne	0.87	0.11	0.75
2,2,5-Trimethylhexane	2.33	1.90	0.43
2,2,6,6-Tetramethylheptane	2.63	2.50	0.13
2,2-Dimethyl-3-hexyne	0.45	-0.08	0.53
2,2-Dimethylheptane	2.32	1.76	0.56
2,2-Dimethylhexane	2.22	1.61	0.61
2,2-Dimethyloctane	2.42	1.91	0.51
2,2-Dimethylpentane	2.11	1.46	0.65
2,2-Dimethylpropane	1.83	1.14	0.69
2,3,4-Trimethylhexane	2.36	1.71	0.65
2,3,4-Trimethylpentane	1.88	1.56	0.32
2,3-Dimethyl-1,3-butadiene	0.29	0.36	-0.07

2,3-Dimethylbutane	1.70	1.09	0.61
2,3-Dimethylheptane	2.34	1.57	0.77
2,3-Dimethylpentane	1.85	1.27	0.58
2,4,6-Trimethyloctane	2.60	2.01	0.59
2,4-Dimethylheptane	2.29	1.57	0.72
2,4-Dimethylhexane	2.16	1.42	0.74
2,4-Dimethylpentane	1.99	1.27	0.72
2,5-Dimethyl-2,4-hexadiene	0.28	0.06	0.22
2,5-Dimethylheptane	2.30	1.57	0.73
2,5-Dimethylhexane	2.17	1.42	0.75
2,6-Dimethylheptane	2.32	1.57	0.75
2,7-Dimethyloctane	2.53	1.72	0.81
2-Heptyne	0.36	-0.60	0.96
2-Methyl-1-pentene	1.08	0.33	0.75
2-Methyl-3-hexyne	0.27	-0.46	0.73
2-Methylheptane	2.15	1.28	0.87
2-Methylhexane	2.11	1.13	0.98
2-Methylpentane	1.84	0.98	0.86
2-Methylpropane	1.65	0.66	0.99
3,3-Dimethylheptane	2.34	1.76	0.57
3,3-Dimethylpentane	1.88	1.46	0.42
3,4-Dimethylhexane	2.22	1.42	0.80
3,5-Dimethylheptane	2.29	1.57	0.72
3-Carene	0.15	-0.36	0.51
3-Ethylheptane	2.33	1.43	0.90
3-Ethylhexane	2.24	1.28	0.96
3-Hexyne	-0.13	-0.66	0.53
3-Isopropylhexane	2.34	1.57	0.76
3-Methyl-1-butene	1.34	0.39	0.95
3-Methylheptane	2.12	1.28	0.84
3-Methylhexane	1.99	1.13	0.86
3-Methylnonane	2.39	1.58	0.81
3-Methylpentane	1.83	0.96	0.87
4,4-Diethylheptane	2.62	2.04	0.58
4,4-Dimethylheptane	2.34	1.76	0.58
4-Ethyl-2-methylhexane	2.30	1.57	0.73
4-Ethylheptane	2.31	1.43	0.88
4-Methyl-1-pentene	1.40	0.45	0.95
4-Methylheptane	2.18	1.28	0.90
4-Methylnonane	2.42	1.58	0.84
4-Methyloctane	2.61	1.43	1.18
4-Propyloctane	2.60	1.73	0.87

4-Vinylcyclohexene	0.26	-0.37	0.63
5-Ethylidene-2-norbornene	-0.32	-1.04	0.72
alpha-Farnesene	0.08	0.31	-0.23
alpha-Humulene	0.14	0.03	0.11
alpha-Neoclovene	0.14	-0.12	0.26
alpha-Phellandrene	0.35	-0.26	0.61
alpha-Pinene	0.74	-0.43	1.17
alpha-Terpinene	-0.15	-0.45	0.30
beta-Phellandrene	0.35	-0.07	0.42
Butane	1.53	0.53	1.00
Camphene	0.23	-0.25	0.48
Caprylene	1.40	0.40	1.00
Cedrene	0.15	-0.22	0.37
cis- Cyclooctene	0.29	-0.56	0.85
cis-1,2-Dimethylcyclohexane	1.17	0.62	0.55
cis-2-Butene	0.98	-0.02	1.00
cis-2-Hexene	1.01	0.10	0.91
cis-2-Octene	1.54	0.22	1.32
cis-2-Pentene	0.96	0.04	0.92
Cyclogeraniolane	1.64	1.10	0.53
Cycloheptane	0.65	0.11	0.54
Cycloheptene	0.28	-0.60	0.88
Cyclohexane	0.88	-0.01	0.89
Cyclohexene	0.07	-0.68	0.75
Cyclooctane	0.74	0.23	0.51
Cyclopentadiene	-0.07	-0.84	0.77
Cyclopentane	0.84	-0.13	0.97
Cyclopentene	0.25	-0.68	0.93
Cyclopropane	0.53	-0.37	0.90
Decane	2.32	1.43	0.89
Diacetylene	-0.66	-1.06	0.40
Diisobutylene	2.00	0.91	1.09
Dodecane	2.53	1.73	0.80
E-beta-Caryophyllene	0.04	-0.06	0.10
Ethane	1.33	0.23	1.10
Ethene	0.83	0.25	0.58
Ethylcyclohexane	1.30	0.48	0.82
Ethyne	-0.01	-0.22	0.21
exo-Dicyclopentadiene	-0.36	-1.46	1.10
gamma-Terpinene	0.02	-0.36	0.38
Heptane	1.96	0.98	0.98
Heptylcyclohexane	1.82	1.23	0.59

Hexane	1.85	0.83	1.02
Isobutene	0.85	0.17	0.68
Isooctane	2.12	1.75	0.37
Isopentane	1.70	0.83	0.87
Isopentene	1.25	0.27	0.98
Isoprene	0.49	0.22	0.27
Isosativene	0.01	-0.33	0.34
Longipinene	0.08	-0.33	0.41
Methylcyclohexane	1.19	0.27	0.92
Methylcyclopentane	1.13	0.15	0.98
Myrcene	0.42	0.40	0.02
Neohexane	1.85	1.29	0.56
Nonane	2.24	1.28	0.96
Nopinene	0.28	-0.25	0.53
Octane	2.07	1.13	0.94
Octylcyclohexane	2.02	1.38	0.64
Pentadecane	2.99	2.18	0.81
Pentane	1.75	0.68	1.07
Pentylcyclopentane	1.87	0.80	1.07
p-Menthane	1.86	1.06	0.80
Propane	1.43	0.38	1.05
Propylcyclohexane	1.62	0.63	0.99
Propylcyclopentane	1.56	0.50	1.06
Propylene	0.86	0.10	0.76
Propyne	-0.27	-0.53	0.26
Sabinene	0.42	-0.15	0.57
s-trans-1,3-Butadiene	0.41	0.15	0.26
Terpinolene	0.03	-0.50	0.53
Tetradecane	2.56	2.03	0.53
trans-1,2-Dimethylcyclohexane	1.39	0.62	0.77
trans-1,3-Dimethylcyclohexane	1.52	0.62	0.90
trans-1,4-Dimethylcyclohexane	1.55	0.62	0.93
trans-2-Butene	0.96	-0.05	1.01
trans-2-Heptene	1.25	0.16	1.09
trans-2-Hexene	1.02	0.10	0.92
trans-2-Octene	1.57	0.22	1.35
trans-2-Pentene	0.98	0.04	0.94
trans-Decalin	0.68	0.14	0.54
Tricyclene	0.92	0.56	0.36
Tridecane	2.07	1.88	0.19
Trimethylethylene	0.98	0.06	0.92
Triptane	2.10	1.60	0.50

Undecane	2.53	1.58	0.95
Valencene	0.10	-0.06	0.16
Vinylacetylene	0.00	-0.43	0.43
Z-Caryophyllene	0.04	-0.06	0.10