3-Buten-2-ol, 2-methyl-

Other names:	1,1-Dimethyl-2-propen-1-ol
	1,1-Dimethyl-2-propenol
	1,1-Dimethyl-2-propenyl alcohol
	1,1-Dimethylallyl alcohol
	1-Buten-3-ol, 3-methyl-
	2-Methyl but-3-ene-2-ol
	2-Methyl-2-hydroxy-3-butene
	2-Methyl-3-buten-2-ol
	2-Methyl-3-buten-2-yl alcohol
	2-Methyl-3-butene-2-ol
	2-Methylbut-3-en-2-ol
	3-Hydroxy-3-methyl-1-butene
	3-Hydroxy-3-methylbutene
	3-Methyl-1-buten-3-ol
	3-Methyl-1-butene-3-ol
	3-Methyl-buten-(1)-ol-(3)
	CH2=CHC(CH3)2OH
	Dimethylvinylcarbinol
	Dimethylvinylmethanol
	NSC 15977
	Vinyldimethylcarbinol
	«alpha»,«alpha»-Dimethylallyl alcohol
	Â«alphaÂ»,Â«alphaÂ»-Dimethylallyl alcohol
Inchi:	InChI=1S/C5H10O/c1-4-5(2,3)6/h4,6H,1H2,2-3H3
InchiKey:	HNVRRHSXBLFLIG-UHFFFAOYSA-N
Formula:	C5H10O
SMILES:	C=CC(C)(C)O
Mol. weight [g/mol]:	86.13
CAS:	115-18-4

Physical Properties

Property code	Value	Unit	Source
chl	-3215.00 ± 0.90	kJ/mol	NIST Webbook
gf	-54.92	kJ/mol	Joback Method
hf	-182.08	kJ/mol	Joback Method
hfl	-181.70 ± 0.90	kJ/mol	NIST Webbook

hfus	0.17	kJ/mol	Comprehensive study of the thermodynamic properties for 2-methyl-3-buten-2-ol
hvap	41.44	kJ/mol	Joback Method
ie	9.90	eV	NIST Webbook
log10ws	-1.14		Crippen Method
logp	0.943		Crippen Method
mcvol	82.880	ml/mol	McGowan Method
pc	4189.32	kPa	Joback Method
rinpol	623.70		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	602.00		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	612.00		NIST Webbook
rinpol	593.00		NIST Webbook
rinpol	593.00		NIST Webbook
rinpol	597.00		NIST Webbook
rinpol	606.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	606.00		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	608.00		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	593.00		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	608.00		NIST Webbook
rinpol	601.00		NIST Webbook
rinpol	603.20		NIST Webbook
rinpol	620.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	620.00		NIST Webbook
rinpol	592.00		NIST Webbook
rinpol	606.00		NIST Webbook
rinpol	602.00		NIST Webbook
ripol	1031.00		NIST Webbook
ripol	1031.00		NIST Webbook
ripol	1037.00		NIST Webbook
ripol	1031.00		NIST Webbook
ripol	1038.00		NIST Webbook
ripol	1051.00		NIST Webbook
ripol	1037.00		NIST Webbook
ripol	1021.00		NIST Webbook

ripol	1035.00		NIST Webbook
ripol	1040.00		NIST Webbook
ripol	1040.00		NIST Webbook
ripol	1036.00		NIST Webbook
ripol	1026.00		NIST Webbook
ripol	1027.00		NIST Webbook
ripol	1026.00		NIST Webbook
ripol	1046.00		NIST Webbook
ripol	1060.00		NIST Webbook
ripol	1026.00		NIST Webbook
ripol	1028.00		NIST Webbook
ripol	1051.00		NIST Webbook
ripol	1036.00		NIST Webbook
ripol	1008.00		NIST Webbook
ripol	1064.00		NIST Webbook
ripol	1058.00		NIST Webbook
ripol	1043.00		NIST Webbook
ripol	1041.00		NIST Webbook
ripol	1075.00		NIST Webbook
ripol	1005.00		NIST Webbook
ripol	1016.00		NIST Webbook
ripol	1038.00		NIST Webbook
ripol	1063.00		NIST Webbook
ripol	1048.00		NIST Webbook
ripol	1064.00		NIST Webbook
ripol	1025.00		NIST Webbook
ripol	1064.00		NIST Webbook
ripol	1048.00		NIST Webbook
ripol	1078.00		NIST Webbook
ripol	1048.00		NIST Webbook
ripol	1035.00		NIST Webbook
ripol	1036.00		NIST Webbook
ripol	1055.00		NIST Webbook
ripol	1023.00		NIST Webbook
ripol	1020.00		NIST Webbook
ripol	1064.00		NIST Webbook
ripol	1022.00		NIST Webbook
ripol	1044.00		NIST Webbook
tb	371.70	K	NIST Webbook
tc	574.89	K	Joback Method
tf	230.15 ± 1.50	K	NIST Webbook
tf	234.15 ± 1.50	K	NIST Webbook
vc	0.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.40	J/mol×K	574.89	Joback Method
cpg	157.15	J/mol×K	399.43	Joback Method
cpg	196.76	J/mol×K	545.65	Joback Method
cpg	189.72	J/mol×K	516.40	Joback Method
cpg	182.26	J/mol×K	487.16	Joback Method
cpg	174.36	J/mol×K	457.92	Joback Method
cpg	166.00	J/mol×K	428.67	Joback Method
cpl	240.70	J/mol×K	298.05	NIST Webbook
cpl	241.20	J/mol×K	298.05	NIST Webbook
dvisc	0.1614936	Pa×s	207.59	Joback Method
dvisc	0.0005920	Pa×s	367.46	Joback Method
dvisc	0.0011851	Pa×s	335.48	Joback Method
dvisc	0.0027461	Pa×s	303.51	Joback Method
dvisc	0.0077559	Pa×s	271.54	Joback Method
dvisc	0.0289005	Pa×s	239.56	Joback Method
dvisc	0.0003305	Pa×s	399.43	Joback Method
hvapt	43.10 ± 0.10	kJ/mol	331.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.34410e+01
Coeff. B	-3.11014e+03
Coeff. C	-4.44690e+01
Temperature range (K), min.	280.92
Temperature range (K), max.	427.04

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C115184&Units=SI

Henry s Law Constants and Infinite Dilution Activity Coefficients of Propane, Propene, Butane, 2-Methylpropane, 1-Butene, 2-Methylpropene, trans-2-Butene, cis-2-Butene, 1,3-Butadiene, Dimethyl Ether, Chloroethane, and 1,1-Difluoroethane in 2-Methyl-3-buten-2-ol and 3-Methyl-3-buten-2-ol:	https://www.doi.org/10.1021/je050343i
Green Leaf Volatiles on Atmospheric Aerosol Particles: A Combined Experimental and Molecular Simulation Study:	https://www.doi.org/10.1021/je500114m
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Comprehensive study of the thermodynamic properties for 2-Methyl-3-buten-2-ol and 3-Methyl-3-buten-2-ol:	https://www.doi.org/10.1016/j.jct.2015.07.028
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume