2-Buten-1-ol, 2-methyl-

Other names:	2-Methyl-2-buten-1-ol
	2-Methyl-2-butenol
	2-Methyl-but-2-ene-1-ol
	2-Methylbut-2-en-1-ol
Inchi:	InChI=1S/C5H10O/c1-3-5(2)4-6/h3,6H,4H2,1-2H3/b5-3-
InchiKey:	NEJDKFPXHQRVMV-HYXAFXHYSA-N
Formula:	C5H10O
SMILES:	CC=C(C)CO
Mol. weight [g/mol]:	86.13
CAS:	4675-87-0

Physical Properties

Property code	Value	Unit	Source
gf	-73.93	kJ/mol	Joback Method
hf	-191.33	kJ/mol	Joback Method
hfus	11.69	kJ/mol	Joback Method
hvap	43.44	kJ/mol	Joback Method
log10ws	-1.03		Crippen Method
logp	0.945		Crippen Method
mcvol	82.880	ml/mol	McGowan Method
pc	4167.71	kPa	Joback Method
rinpol	766.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	754.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1322.00		NIST Webbook
ripol	1322.00		NIST Webbook
ripol	1311.00		NIST Webbook
ripol	1315.00		NIST Webbook
ripol	1324.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1318.00		NIST Webbook
ripol	1332.00		NIST Webbook
ripol	1328.00		NIST Webbook

ripol	1316.00		NIST Webbook
ripol	1309.00		NIST Webbook
ripol	1327.00		NIST Webbook
ripol	1333.00		NIST Webbook
ripol	1315.00		NIST Webbook
ripol	1308.00		NIST Webbook
ripol	1316.00		NIST Webbook
ripol	1325.00		NIST Webbook
ripol	1315.00		NIST Webbook
ripol	1329.00		NIST Webbook
ripol	1333.00		NIST Webbook
ripol	1325.00		NIST Webbook
tb	410.02	K	Joback Method
tc	582.88	K	Joback Method
tf	187.89	K	Joback Method
vc	0.316	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	154.28	J/mol×K	410.02	Joback Method
cpg	162.38	J/mol×K	438.83	Joback Method
cpg	170.11	J/mol×K	467.64	Joback Method
cpg	177.48	J/mol×K	496.45	Joback Method
cpg	184.52	J/mol×K	525.26	Joback Method
cpg	191.23	J/mol×K	554.07	Joback Method
cpg	197.63	J/mol×K	582.88	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.81944e+01
Coeff. B	-4.62916e+03
Coeff. C	-5.60060e+01
Temperature range (K), min.	314.52
Temperature range (K), max.	415.33

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4675870&Units=SI
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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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