

2-methyl-(E)-2-butenol

Inchi:	InChI=1S/C5H10O/c1-3-5(2)4-6/h3,6H,4H2,1-2H3/b5-3+
InchiKey:	NEJDKFPXHQRVMV-HWKANZROSA-N
Formula:	C5H10O
SMILES:	CC=C(C)CO
Mol. weight [g/mol]:	86.13

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
ripol	1322.00		NIST Webbook
ripol	1322.00		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

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R330906&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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