3-Buten-2-ol, 2,3-dimethyl-

Other names: CH2=C(CH3)C(CH3)2OH
2,3-Dimethyl-3-buten-2-ol
2,3-Dimethyl-1-buten-3-ol
3-Hydroxy-2,3-dimethyl-1-butene
2,3-Dimethylbut-3-en-2-ol
Inchi: InChI=1S/C6H12O/c1-5(2)6(3,4)7/h7H,1H2,2-4H3
InchiKey: AWDLBZUXUNIODN-UHFFFAOYSA-N
Formula: C6H12O
SMILES: C=C(C)C(C)(C)O
Mol. weight [g/mol]: 100.16
CAS: 10473-13-9

Physical Properties

Property code	Value	Unit	Source
gf	-55.05	kJ/mol	Joback Method
hf	-212.51	kJ/mol	Joback Method
hfus	5.38	kJ/mol	Joback Method
hvap	43.74	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.333		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3736.23	kPa	Joback Method
rinpol	746.00		NIST Webbook
tb	422.19	K	Joback Method
tc	600.01	K	Joback Method
tf	204.90	K	Joback Method
vc	0.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.48	J/mol×K	422.19	Joback Method
cpg	204.64	J/mol×K	451.83	Joback Method
cpg	214.24	J/mol×K	481.46	Joback Method

cpg	223.33	J/mol×K	511.10	Joback Method
cpg	231.92	J/mol×K	540.73	Joback Method
cpg	240.04	J/mol×K	570.37	Joback Method
cpg	247.71	J/mol×K	600.01	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=C10473139&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume