

5-Hexen-3-ol, 2,3-dimethyl-

Other names:	2,3-Dimethyl-5-hexen-3-ol
Inchi:	InChI=1S/C8H16O/c1-5-6-8(4,9)7(2)3/h5,7,9H,1,6H2,2-4H3
InchiKey:	YGYJSFXFOXFEOD-UHFFFAOYSA-N
Formula:	C8H16O
SMILES:	C=CCC(C)(O)C(C)C
Mol. weight [g/mol]:	128.21
CAS:	19550-90-4

Physical Properties

Property code	Value	Unit	Source
gf	-32.10	kJ/mol	Joback Method
hf	-249.28	kJ/mol	Joback Method
hfus	8.35	kJ/mol	Joback Method
hvap	47.73	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	1.969		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
tb	467.63	K	Joback Method
tc	643.35	K	Joback Method
tf	226.40	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.88	J/mol×K	467.63	Joback Method
cpg	288.18	J/mol×K	496.92	Joback Method
cpg	299.85	J/mol×K	526.20	Joback Method
cpg	310.92	J/mol×K	555.49	Joback Method
cpg	321.41	J/mol×K	584.78	Joback Method
cpg	331.36	J/mol×K	614.06	Joback Method
cpg	340.78	J/mol×K	643.35	Joback Method
dvisc	0.1631928	Pa×s	226.40	Joback Method

dvisc	0.0221752	Pa×s	266.61	Joback Method
dvisc	0.0050841	Pa×s	306.81	Joback Method
dvisc	0.0016398	Pa×s	347.01	Joback Method
dvisc	0.0006690	Pa×s	387.22	Joback Method
dvisc	0.0003231	Pa×s	427.42	Joback Method
dvisc	0.0001768	Pa×s	467.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19550904&Units=SI
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
dvisc:	Dynamic viscosity
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
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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