

5-Methyl-5-hexen-3-ol

Inchi:	InChI=1S/C7H14O/c1-4-7(8)5-6(2)3/h7-8H,2,4-5H2,1,3H3
InchiKey:	LZJQEGCYVOMQID-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	C=C(C)CC(O)CC
Mol. weight [g/mol]:	114.19
CAS:	67760-89-8

Physical Properties

Property code	Value	Unit	Source
gf	-51.91	kJ/mol	Joback Method
hf	-229.68	kJ/mol	Joback Method
hfus	11.86	kJ/mol	Joback Method
hvap	46.88	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.723		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
tb	447.86	K	Joback Method
tc	617.74	K	Joback Method
tf	198.75	K	Joback Method
vc	0.422	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.50	J/mol×K	447.86	Joback Method
cpg	241.95	J/mol×K	476.17	Joback Method
cpg	251.95	J/mol×K	504.49	Joback Method
cpg	261.54	J/mol×K	532.80	Joback Method
cpg	270.72	J/mol×K	561.11	Joback Method
cpg	279.50	J/mol×K	589.43	Joback Method
cpg	287.90	J/mol×K	617.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67760898&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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

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