2,5-Dimethyl-5-hexen-3-ol

Inchi: InChI=1S/C8H16O/c1-6(2)5-8(9)7(3)4/h7-9H,1,5H2,2-4H3
InchiKey: LCBOFRBFVBROGF-UHFFFAOYSA-N
Formula: C8H16O
SMILES: C=C(C)CC(O)C(C)C
Mol. weight [g/mol]: 128.21
CAS: 67760-91-2

Physical Properties

Property code	Value	Unit	Source
gf	-45.93	kJ/mol	Joback Method
hf	-255.60	kJ/mol	Joback Method
hfus	10.93	kJ/mol	Joback Method
hvap	48.72	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	1.969		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
tb	470.30	K	Joback Method
tc	642.58	K	Joback Method
tf	195.02	K	Joback Method
vc	0.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.13	J/mol×K	470.30	Joback Method
cpg	284.90	J/mol×K	499.01	Joback Method
cpg	296.15	J/mol×K	527.73	Joback Method
cpg	306.92	J/mol×K	556.44	Joback Method
cpg	317.22	J/mol×K	585.15	Joback Method
cpg	327.06	J/mol×K	613.87	Joback Method
cpg	336.46	J/mol×K	642.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67760912&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
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