2-Methyl-1-hepten-3-ol

Inchi: InChI=1S/C8H16O/c1-4-5-6-8(9)7(2)3/h8-9H,2,4-6H2,1,3H3
InchiKey: PPKIOOAEILEYAF-UHFFFAOYSA-N
Formula: C8H16O
SMILES: C=C(C)C(O)CCCC
Mol. weight [g/mol]: 128.21
CAS: 13019-19-7

Physical Properties

Property code	Value	Unit	Source
gf	-43.49	kJ/mol	Joback Method
hf	-250.32	kJ/mol	Joback Method
hfus	14.45	kJ/mol	Joback Method
hvap	49.10	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.114		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2956.90	kPa	Joback Method
rinpol	959.00		NIST Webbook
rinpol	961.00		NIST Webbook
rinpol	961.00		NIST Webbook
rinpol	960.00		NIST Webbook
tb	470.74	K	Joback Method
tc	639.51	K	Joback Method
tf	210.02	K	Joback Method
vc	0.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.97	J/mol×K	470.74	Joback Method
cpg	284.42	J/mol×K	498.87	Joback Method
cpg	295.40	J/mol×K	527.00	Joback Method
cpg	305.91	J/mol×K	555.13	Joback Method
cpg	315.97	J/mol×K	583.25	Joback Method

cpg	325.60	J/mol×K	611.38	Joback Method
cpg	334.81	J/mol×K	639.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13019197&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume