6-Hepten-2-ol, 2,6-dimethyl-

Inchi: InChI=1S/C9H18O/c1-8(2)6-5-7-9(3,4)10/h10H,1,5-7H2,2-4H3
InchiKey: ICHVSYBMEODCOO-UHFFFAOYSA-N
Formula: C9H18O
SMILES: C=C(C)CCCC(C)(C)O
Mol. weight [g/mol]: 142.24
CAS: 32779-58-1

Physical Properties

Property code	Value	Unit	Source
gf	-29.79	kJ/mol	Joback Method
hf	-274.43	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	50.42	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.504		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	995.70		NIST Webbook
tb	490.83	K	Joback Method
tc	664.56	K	Joback Method
tf	238.71	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.24	J/mol×K	490.83	Joback Method
cpg	332.23	J/mol×K	519.79	Joback Method
cpg	344.58	J/mol×K	548.74	Joback Method
cpg	356.31	J/mol×K	577.70	Joback Method
cpg	367.44	J/mol×K	606.65	Joback Method
cpg	378.02	J/mol×K	635.61	Joback Method
cpg	388.06	J/mol×K	664.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32779581&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume