3,6-Dimethyl-6-hepten-4-yn-3-ol

Inchi: InChI=1S/C9H14O/c1-5-9(4,10)7-6-8(2)3/h10H,2,5H2,1,3-4H3
InchiKey: VSSPEZDVPCUEIR-UHFFFAOYSA-N
Formula: C9H14O
SMILES: C=C(C)C#CC(C)(O)CC
Mol. weight [g/mol]: 138.21
CAS: 3601-67-0

Physical Properties

Property code	Value	Unit	Source
gf	173.01	kJ/mol	Joback Method
hf	-2.13	kJ/mol	Joback Method
hfus	16.27	kJ/mol	Joback Method
hvap	52.57	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	1.727		Crippen Method
mcvol	130.640	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
tb	499.83	K	Joback Method
tc	695.63	K	Joback Method
tf	344.81	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.42	J/mol×K	499.83	Joback Method
cpg	298.46	J/mol×K	532.46	Joback Method
cpg	309.81	J/mol×K	565.10	Joback Method
cpg	320.52	J/mol×K	597.73	Joback Method
cpg	330.62	J/mol×K	630.37	Joback Method
cpg	340.15	J/mol×K	663.00	Joback Method
cpg	349.14	J/mol×K	695.63	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3601670&Units=SI

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