4-Methyl-2-octyn-4-ol

Inchi: InChI=1S/C9H16O/c1-4-6-8-9(3,10)7-5-2/h10H,4,6,8H2,1-3H3
InchiKey: HWVNLGPDLREHJB-UHFFFAOYSA-N
Formula: C9H16O
SMILES: CC#CC(C)(O)CCCC
Mol. weight [g/mol]: 140.23

Physical Properties

Property code	Value	Unit	Source
af	0.5538		Cheméo Relay (1.0)
gf	93.72	kJ/mol	Joback Method
hf	-109.00	kJ/mol	Cheméo Relay (1.0)
hfus	18.86	kJ/mol	Joback Method
hvap	66.91	kJ/mol	Cheméo Relay (1.0)
ie	9.63	eV	Cheméo Relay (1.0)
log10ws	-1.58		Cheméo Relay (1.0)
logp	1.951		Crippen Method
mcvol	134.940	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
tb	448.89	K	Cheméo Relay (1.0)
tc	646.33	K	Cheméo Relay (1.0)
tf	256.85	K	Cheméo Relay (1.0)
vc	0.482	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.46	J/mol×K	503.27	Joback Method
cpg	316.95	J/mol×K	534.67	Joback Method
cpg	328.80	J/mol×K	566.08	Joback Method
cpg	340.04	J/mol×K	597.48	Joback Method
cpg	350.69	J/mol×K	628.89	Joback Method
cpg	360.79	J/mol×K	660.29	Joback Method
cpg	370.37	J/mol×K	691.70	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74514593&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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