6-Methyl-6-hepten-4-yn-3-ol

Inchi: InChI=1S/C8H12O/c1-4-8(9)6-5-7(2)3/h8-9H,2,4H2,1,3H3
InchiKey: DUDZQARPXNGCOB-UHFFFAOYSA-N
Formula: C8H12O
SMILES: C=C(C)C#CC(O)CC
Mol. weight [g/mol]: 124.18
CAS: 95764-76-4

Physical Properties

Property code	Value	Unit	Source
gf	159.31	kJ/mol	Joback Method
hf	21.98	kJ/mol	Joback Method
hfus	17.57	kJ/mol	Joback Method
hvap	51.25	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.337		Crippen Method
mcvol	116.550	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
rinpol	972.00		NIST Webbook
rinpol	972.00		NIST Webbook
tb	479.74	K	Joback Method
tc	670.27	K	Joback Method
tf	316.12	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.27	J/mol×K	479.74	Joback Method
cpg	251.64	J/mol×K	511.49	Joback Method
cpg	261.53	J/mol×K	543.25	Joback Method
cpg	270.95	J/mol×K	575.00	Joback Method
cpg	279.94	J/mol×K	606.76	Joback Method
cpg	288.50	J/mol×K	638.51	Joback Method
cpg	296.64	J/mol×K	670.27	Joback Method

Sources

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=C95764764&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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