4-Methyl-2-heptyn-4-ol

Inchi: InChI=1S/C8H14O/c1-4-6-8(3,9)7-5-2/h9H,4,6H2,1-3H3
InchiKey: ZGPJPUGCDODKKH-UHFFFAOYSA-N
Formula: C8H14O
SMILES: CC#CC(C)(O)CCC
Mol. weight [g/mol]: 126.20
CAS: 4376-16-3

Physical Properties

Property code	Value	Unit	Source
gf	85.30	kJ/mol	Joback Method
hf	-97.13	kJ/mol	Joback Method
hfus	16.27	kJ/mol	Joback Method
hvap	50.94	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	1.561		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
tb	480.39	K	Joback Method
tc	671.00	K	Joback Method
tf	349.26	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.45	J/mol×K	480.39	Joback Method
cpg	272.99	J/mol×K	512.16	Joback Method
cpg	283.92	J/mol×K	543.93	Joback Method
cpg	294.28	J/mol×K	575.69	Joback Method
cpg	304.09	J/mol×K	607.46	Joback Method
cpg	313.38	J/mol×K	639.23	Joback Method
cpg	322.18	J/mol×K	671.00	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=C4376163&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume