3-Methyl-6-hepten-1-yn-3-ol

Inchi: InChI=1S/C8H12O/c1-4-6-7-8(3,9)5-2/h2,4,9H,1,6-7H2,3H3
InchiKey: PVJVUJJZSINIGV-UHFFFAOYSA-N
Formula: C8H12O
SMILES: C#CC(C)(O)CCC=C
Mol. weight [g/mol]: 124.18
CAS: 51193-99-8

Physical Properties

Property code	Value	Unit	Source
gf	193.41	kJ/mol	Joback Method
hf	47.90	kJ/mol	Joback Method
hfus	14.84	kJ/mol	Joback Method
hvap	47.97	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.337		Crippen Method
mcvol	116.550	ml/mol	McGowan Method
pc	3522.09	kPa	Joback Method
tb	458.19	K	Joback Method
tc	641.88	K	Joback Method
tf	288.37	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.84	J/mol×K	458.19	Joback Method
cpg	255.44	J/mol×K	488.80	Joback Method
cpg	265.41	J/mol×K	519.42	Joback Method
cpg	274.79	J/mol×K	550.03	Joback Method
cpg	283.60	J/mol×K	580.65	Joback Method
cpg	291.89	J/mol×K	611.26	Joback Method
cpg	299.68	J/mol×K	641.88	Joback Method

Sources

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=C51193998&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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