3,6-Dimethyl-1-heptyn-3-ol

Other names: 1-Heptyn-3-ol, 3,6-dimethyl-
Inchi: InChI=1S/C9H16O/c1-5-9(4,10)7-6-8(2)3/h1,8,10H,6-7H2,2-4H3
InchiKey: COWFALGRNJAHKW-UHFFFAOYSA-N
Formula: C9H16O
SMILES: C#CC(C)(O)CCC(C)C
Mol. weight [g/mol]: 140.22
CAS: 19549-98-5

Physical Properties

Property code	Value	Unit	Source
gf	111.55	kJ/mol	Joback Method
hf	-103.45	kJ/mol	Joback Method
hfus	15.19	kJ/mol	Joback Method
hvap	50.48	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	1.807		Crippen Method
mcvol	134.940	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
tb	483.95	K	Joback Method
tc	666.13	K	Joback Method
tf	286.40	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.93	J/mol×K	483.95	Joback Method
cpg	316.40	J/mol×K	514.31	Joback Method
cpg	328.20	J/mol×K	544.68	Joback Method
cpg	339.36	J/mol×K	575.04	Joback Method
cpg	349.91	J/mol×K	605.41	Joback Method
cpg	359.89	J/mol×K	635.77	Joback Method
cpg	369.32	J/mol×K	666.13	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	332.50 ± 0.50	K	0.70	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19549985&Units=SI
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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume