3-Methyl-1-nonyne-3-ol

Other names: 3-Methyl-1-nonyn-3-ol
3-Methyl-1-nonyne-3-ol
Inchi: InChI=1S/C10H18O/c1-4-6-7-8-9-10(3,11)5-2/h2,11H,4,6-9H2,1,3H3
InchiKey: VQUXVWMAXIQKTQ-UHFFFAOYSA-N
Formula: C10H18O
SMILES: C#CC(C)(O)CCCCCC
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
af	0.6052		Cheméo Relay (1.0)
gf	122.41	kJ/mol	Joback Method
hf	-153.90	kJ/mol	Cheméo Relay (1.0)
hfus	21.30	kJ/mol	Joback Method
hvap	69.39	kJ/mol	Cheméo Relay (1.0)
ie	10.08	eV	Cheméo Relay (1.0)
log10ws	-2.61		Cheméo Relay (1.0)
logp	2.341		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
tb	463.34	K	Cheméo Relay (1.0)
tc	649.83	K	Cheméo Relay (1.0)
tf	270.84	K	Cheméo Relay (1.0)
vc	0.539	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.97	J/mol×K	507.27	Joback Method
cpg	360.93	J/mol×K	536.73	Joback Method
cpg	373.22	J/mol×K	566.20	Joback Method
cpg	384.88	J/mol×K	595.66	Joback Method
cpg	395.93	J/mol×K	625.13	Joback Method
cpg	406.42	J/mol×K	654.59	Joback Method

cpg	416.37	J/mol×K	684.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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=C5430013&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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