3-Ethyl-5-methyl-1-heptyn-3-ol

Inchi: InChI=1S/C10H18O/c1-5-9(4)8-10(11,6-2)7-3/h2,9,11H,5,7-8H2,1,3-4H3
InchiKey: FMLRBVOUYLRDRV-UHFFFAOYSA-N
Formula: C10H18O
SMILES: C#CC(O)(CC)CC(C)CC
Mol. weight [g/mol]: 154.25
CAS: 207974-16-1

Physical Properties

Property code	Value	Unit	Source
gf	119.97	kJ/mol	Joback Method
hf	-124.09	kJ/mol	Joback Method
hfus	17.78	kJ/mol	Joback Method
hvap	52.71	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.197		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
tb	506.83	K	Joback Method
tc	687.22	K	Joback Method
tf	297.67	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.20	J/mol×K	506.83	Joback Method
cpg	361.50	J/mol×K	536.89	Joback Method
cpg	374.09	J/mol×K	566.96	Joback Method
cpg	386.01	J/mol×K	597.02	Joback Method
cpg	397.30	J/mol×K	627.09	Joback Method
cpg	407.99	J/mol×K	657.15	Joback Method
cpg	418.12	J/mol×K	687.22	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C207974161&Units=SI

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