3-Isopropyl-4-methyl-1-pentyn-3-ol

Inchi: InChI=1S/C9H16O/c1-6-9(10,7(2)3)8(4)5/h1,7-8,10H,2-5H3
InchiKey: DIFXCBNNWBBNCA-UHFFFAOYSA-N
Formula: C9H16O
SMILES: C#CC(O)(C(C)C)C(C)C
Mol. weight [g/mol]: 140.22
CAS: 5333-87-9

Physical Properties

Property code	Value	Unit	Source
gf	109.11	kJ/mol	Joback Method
hf	-108.73	kJ/mol	Joback Method
hfus	11.67	kJ/mol	Joback Method
hvap	50.09	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	1.663		Crippen Method
mcvol	134.940	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
tb	483.51	K	Joback Method
tc	669.62	K	Joback Method
tf	271.40	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.12	J/mol×K	483.51	Joback Method
cpg	316.93	J/mol×K	514.53	Joback Method
cpg	329.04	J/mol×K	545.55	Joback Method
cpg	340.48	J/mol×K	576.57	Joback Method
cpg	351.27	J/mol×K	607.58	Joback Method
cpg	361.45	J/mol×K	638.60	Joback Method
cpg	371.07	J/mol×K	669.62	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=C5333879&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