1-Ethynylcyclopentanol

Other names: 1-Ethynyl-1-cyclopentanol
Cyclopentanol, 1-ethynyl-
Inchi: InChI=1S/C7H10O/c1-2-7(8)5-3-4-6-7/h1,8H,3-6H2
InchiKey: LQMDOONLLAJAPZ-UHFFFAOYSA-N
Formula: C7H10O
SMILES: C#CC1(O)CCCC1
Mol. weight [g/mol]: 110.15
CAS: 17356-19-3

Physical Properties

Property code	Value	Unit	Source
gf	125.37	kJ/mol	Joback Method
hf	27.58	kJ/mol	Joback Method
hfus	8.59	kJ/mol	Joback Method
hvap	62.10	kJ/mol	NIST Webbook
log10ws	-1.82		Crippen Method
logp	0.925		Crippen Method
mcvol	95.900	ml/mol	McGowan Method
pc	4924.59	kPa	Joback Method
tb	430.00	K	NIST Webbook
tb	430.70	K	NIST Webbook
tc	665.22	K	Joback Method
tf	311.24	K	Joback Method
vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.99	J/mol×K	457.38	Joback Method
cpg	212.70	J/mol×K	492.02	Joback Method
cpg	223.46	J/mol×K	526.66	Joback Method
cpg	233.37	J/mol×K	561.30	Joback Method
cpg	242.55	J/mol×K	595.94	Joback Method
cpg	251.10	J/mol×K	630.58	Joback Method

cpg	259.14	J/mol×K	665.22	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=C17356193&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