1-Ethynyl-1-cycloheptanol

Other names: 1-Ethynylcycloheptanol
Inchi: InChI=1S/C9H14O/c1-2-9(10)7-5-3-4-6-8-9/h1,10H,3-8H2
InchiKey: QKJJSXGDSZZUKI-UHFFFAOYSA-N
Formula: C9H14O
SMILES: C#CC1(O)CCCCCC1
Mol. weight [g/mol]: 138.21
CAS: 2809-78-1

Physical Properties

Property code	Value	Unit	Source
gf	118.01	kJ/mol	Joback Method
hf	-26.02	kJ/mol	Joback Method
hfus	9.57	kJ/mol	Joback Method
hvap	51.62	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	1.705		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	4072.51	kPa	Joback Method
tb	511.68	K	Joback Method
tc	729.36	K	Joback Method
tf	326.74	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.24	J/mol×K	511.68	Joback Method
cpg	300.45	J/mol×K	547.96	Joback Method
cpg	314.61	J/mol×K	584.24	Joback Method
cpg	327.84	J/mol×K	620.52	Joback Method
cpg	340.25	J/mol×K	656.80	Joback Method
cpg	351.95	J/mol×K	693.08	Joback Method
cpg	363.06	J/mol×K	729.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2809781&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume