Cyclopropane, 1-ethynyl-1-(1-propynyl-

Inchi: InChI=1S/C8H8/c1-3-5-8(4-2)6-7-8/h2H,6-7H2,1H3
InchiKey: CRUULDHEGJSVDL-UHFFFAOYSA-N
Formula: C8H8
SMILES: C#CC1(C#CC)CC1
Mol. weight [g/mol]: 104.15
CAS: 105961-79-3

Physical Properties

Property code	Value	Unit	Source
gf	497.61	kJ/mol	Joback Method
hf	443.79	kJ/mol	Joback Method
hfus	14.41	kJ/mol	Joback Method
hvap	34.17	kJ/mol	Joback Method
ie	8.88	eV	NIST Webbook
log10ws	-2.41		Crippen Method
logp	1.423		Crippen Method
mcvol	95.520	ml/mol	McGowan Method
pc	4426.72	kPa	Joback Method
tb	388.54	K	Joback Method
tc	619.54	K	Joback Method
tf	374.83	K	Joback Method
vc	0.362	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.70	J/mol×K	388.54	Joback Method
cpg	180.44	J/mol×K	427.04	Joback Method
cpg	191.83	J/mol×K	465.54	Joback Method
cpg	202.04	J/mol×K	504.04	Joback Method
cpg	211.22	J/mol×K	542.54	Joback Method
cpg	219.55	J/mol×K	581.04	Joback Method
cpg	227.19	J/mol×K	619.54	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=C105961793&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
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