Cyclohexene,1-ethynyl-

Other names: 1-ethynyl-1-cyclohexene
Inchi: InChI=1S/C8H10/c1-2-8-6-4-3-5-7-8/h1,6H,3-5,7H2
InchiKey: DKFHWNGVMWFBJE-UHFFFAOYSA-N
Formula: C8H10
SMILES: C#CC1=CCCCC1
Mol. weight [g/mol]: 106.17
CAS: 931-49-7

Physical Properties

Property code	Value	Unit	Source
gf	292.04	kJ/mol	Joback Method
hf	204.42	kJ/mol	Joback Method
hfus	11.05	kJ/mol	Joback Method
hvap	34.95	kJ/mol	Joback Method
ie	8.61 ± 0.01	eV	NIST Webbook
log10ws	-2.71		Crippen Method
logp	2.120		Crippen Method
mcvol	99.820	ml/mol	McGowan Method
pc	4010.84	kPa	Joback Method
rinpol	862.00		NIST Webbook
tb	422.70	K	NIST Webbook
tc	622.23	K	Joback Method
tf	251.79	K	Joback Method
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.90	J/mol×K	400.92	Joback Method
cpg	188.80	J/mol×K	437.80	Joback Method
cpg	201.87	J/mol×K	474.69	Joback Method
cpg	214.14	J/mol×K	511.57	Joback Method
cpg	225.64	J/mol×K	548.46	Joback Method
cpg	236.42	J/mol×K	585.34	Joback Method

cpg	246.51	J/mol×K	622.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C931497&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume