

Cyclohexylacetylene

Other names:	Cyclohexylethyne Cyclohexane, ethynyl- ethynylcyclohexane
Inchi:	InChI=1S/C8H12/c1-2-8-6-4-3-5-7-8/h1,8H,3-7H2
InchiKey:	SSDZYLQUYMOSAK-UHFFFAOYSA-N
Formula:	C8H12
SMILES:	C#CC1CCCCC1
Mol. weight [g/mol]:	108.18
CAS:	931-48-6

Physical Properties

Property code	Value	Unit	Source
gf	264.00	kJ/mol	Joback Method
hf	137.77	kJ/mol	Joback Method
hfus	11.29	kJ/mol	Joback Method
hvap	33.69	kJ/mol	Joback Method
ie	9.92	eV	NIST Webbook
log10ws	-2.62		Crippen Method
logp	2.200		Crippen Method
mcvol	104.120	ml/mol	McGowan Method
pc	3749.97	kPa	Joback Method
tb	392.11	K	Joback Method
tc	608.79	K	Joback Method
tf	234.27	K	Joback Method
vc	0.379	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.01	J/mol×K	392.11	Joback Method
cpg	202.19	J/mol×K	428.22	Joback Method
cpg	217.47	J/mol×K	464.34	Joback Method
cpg	231.88	J/mol×K	500.45	Joback Method
cpg	245.46	J/mol×K	536.56	Joback Method

cpg	258.23	J/mol×K	572.68	Joback Method
cpg	270.23	J/mol×K	608.79	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=C931486&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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