Cyclopropylacethylene

Other names: Cyclopropane,ethynyl-
Cyclopropylacethylene
ethynyl cyclopropane
Inchi: InChI=1S/C5H6/c1-2-5-3-4-5/h1,5H,3-4H2
InchiKey: NPTDXPDGUHAFKC-UHFFFAOYSA-N
Formula: C5H6
SMILES: C#CC1CC1
Mol. weight [g/mol]: 66.10

Physical Properties

Property code	Value	Unit	Source
chl	-3086.10 ± 0.80	kJ/mol	NIST Webbook
hf	292.00 ± 1.60	kJ/mol	NIST Webbook
hfl	261.10 ± 0.80	kJ/mol	NIST Webbook
hfus	9.82	kJ/mol	Joback Method
hvap	30.90 ± 1.50	kJ/mol	NIST Webbook
hvap	30.90	kJ/mol	NIST Webbook
ie	8.70	eV	NIST Webbook
ie	9.58	eV	NIST Webbook
logp	1.030		Crippen Method
mcvol	61.850	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	88.50	J/mol×K	310.66	Joback Method
cpg	97.63	J/mol×K	342.63	Joback Method
cpg	106.16	J/mol×K	374.60	Joback Method
cpg	114.12	J/mol×K	406.57	Joback Method
cpg	121.55	J/mol×K	438.54	Joback Method
cpg	128.48	J/mol×K	470.51	Joback Method
cpg	134.93	J/mol×K	502.49	Joback Method
hvapt	31.10	kJ/mol	305.00	NIST Webbook

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6746947&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume