Cyclopropane, 1,1-diethynyl-

Inchi: InChI=1S/C7H6/c1-3-7(4-2)5-6-7/h1-2H,5-6H2
InchiKey: NYLVKOBKPNQZTK-UHFFFAOYSA-N
Formula: C7H6
SMILES: C#CC1(C#C)CC1
Mol. weight [g/mol]: 90.12
CAS: 72323-66-1

Physical Properties

Property code	Value	Unit	Source
chl	-4113.00 ± 0.80	kJ/mol	NIST Webbook
gf	509.46	kJ/mol	Joback Method
hf	538.50 ± 1.20	kJ/mol	NIST Webbook
hfl	500.90 ± 1.20	kJ/mol	NIST Webbook
hfus	11.67	kJ/mol	Joback Method
hvap	37.60	kJ/mol	NIST Webbook
hvap	37.60	kJ/mol	NIST Webbook
ie	8.90	eV	NIST Webbook
ie	9.26	eV	NIST Webbook
log10ws	-1.99		Crippen Method
logp	1.033		Crippen Method
mcvol	81.430	ml/mol	McGowan Method
pc	4966.33	kPa	Joback Method
tb	373.00 ± 0.30	K	NIST Webbook
tc	563.60	K	Joback Method
tf	304.43	K	Joback Method
vc	0.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	132.83	J/mol×K	346.78	Joback Method
cpg	144.48	J/mol×K	382.92	Joback Method
cpg	154.76	J/mol×K	419.05	Joback Method
cpg	163.83	J/mol×K	455.19	Joback Method

cpg	171.83	J/mol×K	491.33	Joback Method
cpg	178.90	J/mol×K	527.46	Joback Method
cpg	185.19	J/mol×K	563.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72323661&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

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
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
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