

Cyclopropane, 1-ethynyl-1-ethenyl-

Inchi:	InChI=1S/C7H8/c1-3-7(4-2)5-6-7/h1,4H,2,5-6H2
InchiKey:	TYVGPCXTPUBRCP-UHFFFAOYSA-N
Formula:	C7H8
SMILES:	C#CC1(C=C)CC1
Mol. weight [g/mol]:	92.14
CAS:	105961-74-8

Physical Properties

Property code	Value	Unit	Source
gf	374.23	kJ/mol	Joback Method
hf	317.56	kJ/mol	Joback Method
hfus	7.42	kJ/mol	Joback Method
hvap	29.13	kJ/mol	Joback Method
ie	8.60	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
log10ws	-2.05		Crippen Method
logp	1.586		Crippen Method
mcvol	85.730	ml/mol	McGowan Method
pc	4299.92	kPa	Joback Method
tb	353.34	K	Joback Method
tc	558.71	K	Joback Method
tf	255.70	K	Joback Method
vc	0.326	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	140.98	J/mol×K	353.34	Joback Method
cpg	153.64	J/mol×K	387.57	Joback Method
cpg	165.02	J/mol×K	421.80	Joback Method
cpg	175.26	J/mol×K	456.02	Joback Method
cpg	184.47	J/mol×K	490.25	Joback Method
cpg	192.78	J/mol×K	524.48	Joback Method
cpg	200.30	J/mol×K	558.71	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=C105961748&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

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