

Cyclopropene, 3-methyl-3-vinyl-

Inchi:

InChI=1S/C6H8/c1-3-6(2)4-5-6/h3-5H,1H2,2H3

InchiKey:

AZGBUFPIKVKSCD-UHFFFAOYSA-N

Formula:

C6H8

SMILES:

C=CC1(C)C=C1

Mol. weight [g/mol]:

80.13

CAS:

71153-30-5

Physical Properties

Property code	Value	Unit	Source
gf	172.70	kJ/mol	Joback Method
hf	104.08	kJ/mol	Joback Method
hfus	3.08	kJ/mol	Joback Method
hvap	27.33	kJ/mol	Joback Method
ie	8.29	eV	NIST Webbook
log10ws	-1.69		Crippen Method
logp	1.748		Crippen Method
mcvol	75.940	ml/mol	McGowan Method
pc	4211.09	kPa	Joback Method
tb	339.50	K	Joback Method
tc	532.66	K	Joback Method
tf	198.22	K	Joback Method
vc	0.293	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	117.26	J/mol×K	339.50	Joback Method
cpg	129.00	J/mol×K	371.69	Joback Method
cpg	139.64	J/mol×K	403.89	Joback Method
cpg	149.27	J/mol×K	436.08	Joback Method
cpg	157.99	J/mol×K	468.27	Joback Method
cpg	165.90	J/mol×K	500.47	Joback Method
cpg	173.09	J/mol×K	532.66	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=C71153305&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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