Isopropenylcyclopropane

Other names:	Cyclopropane, (1-methylethenyl)-
	Propene, 2-cyclopropyl-
	2-Cyclopropyl-1-propene
	2-Cyclopropylpropene
	1-Methylethenylcyclopropane
	Isopropneylcyclopropane
Inchi:	InChI=1S/C6H10/c1-5(2)6-3-4-6/h6H,1,3-4H2,2H3
InchiKey:	MKPHNILWOMCVTH-UHFFFAOYSA-N
Formula:	C6H10
SMILES:	C=C(C)C1CC1
Mol. weight [g/mol]:	82.14
CAS:	4663-22-3

Physical Properties

Property code	Value	Unit	Source
affp	871.60	kJ/mol	NIST Webbook
basg	842.70	kJ/mol	NIST Webbook
chl	-3620.00	kJ/mol	NIST Webbook
chl	-3849.00	kJ/mol	NIST Webbook
gf	139.68	kJ/mol	Joback Method
hf	21.27	kJ/mol	Joback Method
hfus	6.84	kJ/mol	Joback Method
hvap	28.27	kJ/mol	Joback Method
ie	8.66 ± 0.05	eV	NIST Webbook
ie	9.12	eV	NIST Webbook
log10ws	-1.84		Crippen Method
logp	1.973		Crippen Method
mcvol	80.240	ml/mol	McGowan Method
pc	3824.55	kPa	Joback Method
rinpol	617.00		NIST Webbook
rinpol	619.00		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	616.00		NIST Webbook
tb	339.98	K	Joback Method
tc	526.23	K	Joback Method
tf	170.81 ± 0.15	K	NIST Webbook

tf	170.79 ± 0.20	K	NIST Webbook
tf	170.81 ± 0.30	K	NIST Webbook
tf	170.81 ± 0.20	K	NIST Webbook
vc	0.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	127.75	J/mol×K	339.98	Joback Method
cpg	139.63	J/mol×K	371.02	Joback Method
cpg	150.84	J/mol×K	402.06	Joback Method
cpg	161.41	J/mol×K	433.10	Joback Method
cpg	171.37	J/mol×K	464.14	Joback Method
cpg	180.75	J/mol×K	495.19	Joback Method
cpg	189.59	J/mol×K	526.23	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=C4663223&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume