1,1'-Bicyclopropyl

Other names:	Bicyclopropyl
	Cyclopropane, cyclopropyl-
Inchi:	InChI=1S/C6H10/c1-2-5(1)6-3-4-6/h5-6H,1-4H2
InchiKey:	PGPFRBIKUWKSTJ-UHFFFAOYSA-N
Formula:	C6H10
SMILES:	C1CC1C1CC1
Mol. weight [g/mol]:	82.14
CAS:	5685-46-1

Physical Properties

Property code	Value	Unit	Source
chl	-3886.10 ± 3.30	kJ/mol	NIST Webbook
gf	121.14	kJ/mol	Joback Method
hf	130.00 ± 5.00	kJ/mol	NIST Webbook
hfl	96.00 ± 3.80	kJ/mol	NIST Webbook
hfus	7.57	kJ/mol	Joback Method
hvap	34.00	kJ/mol	NIST Webbook
hvap	33.00 ± 1.00	kJ/mol	NIST Webbook
hvap	31.70 ± 0.50	kJ/mol	NIST Webbook
ie	9.04	eV	NIST Webbook
ie	8.80 ± 0.02	eV	NIST Webbook
ie	9.50	eV	NIST Webbook
ie	9.12 ± 0.05	eV	NIST Webbook
ie	8.90	eV	NIST Webbook
ie	9.60	eV	NIST Webbook
log10ws	-1.64		Crippen Method
logp	1.806		Crippen Method
mcvol	73.680	ml/mol	McGowan Method
pc	4249.61	kPa	Joback Method
rinpol	646.20		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	640.20		NIST Webbook
rinpol	640.20		NIST Webbook
tb	349.25 ± 0.40	K	NIST Webbook
tc	545.42	K	Joback Method
tf	190.53 ± 0.30	K	NIST Webbook
vc	0.285	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	123.56	J/mol×K	350.16	Joback Method
cpg	137.73	J/mol×K	382.70	Joback Method
cpg	150.96	J/mol×K	415.25	Joback Method
cpg	163.29	J/mol×K	447.79	Joback Method
cpg	174.79	J/mol×K	480.33	Joback Method
cpg	185.50	J/mol×K	512.88	Joback Method
cpg	195.48	J/mol×K	545.42	Joback Method
dvisc	0.0002505	Pa×s	193.26	Joback Method
dvisc	0.0002758	Pa×s	219.41	Joback Method
dvisc	0.0002976	Pa×s	245.56	Joback Method
dvisc	0.0003163	Pa×s	271.71	Joback Method
dvisc	0.0003327	Pa×s	297.86	Joback Method
dvisc	0.0003471	Pa×s	324.01	Joback Method
dvisc	0.0003599	Pa×s	350.16	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5685461&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume