

1,1'-Bicyclopropyl, 1,1'-dimethyl-

Other names:	1,1'-Dimethyl bicyclopropyl
Inchi:	InChI=1S/C8H14/c1-7(3-4-7)8(2)5-6-8/h3-6H2,1-2H3
InchiKey:	UEKMEJJABUQZMZ-UHFFFAOYSA-N
Formula:	C8H14
SMILES:	CC1(C2(C)CC2)CC1
Mol. weight [g/mol]:	110.20
CAS:	59020-33-6

Physical Properties

Property code	Value	Unit	Source
gf	127.00	kJ/mol	Joback Method
hf	-32.37	kJ/mol	Joback Method
hfus	0.15	kJ/mol	Joback Method
hvap	30.93	kJ/mol	Joback Method
ie	9.30	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
log10ws	-2.48		Crippen Method
logp	2.587		Crippen Method
mcvol	101.860	ml/mol	McGowan Method
pc	3736.23	kPa	Joback Method
tb	396.40	K	Joback Method
tc	607.93	K	Joback Method
tf	263.60	K	Joback Method
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.49	J/mol×K	396.40	Joback Method
cpg	220.62	J/mol×K	431.65	Joback Method
cpg	236.81	J/mol×K	466.91	Joback Method
cpg	251.29	J/mol×K	502.16	Joback Method
cpg	264.30	J/mol×K	537.42	Joback Method
cpg	276.06	J/mol×K	572.67	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C59020336&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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