Bicyclo[2.2.2]octane, 2-chloro-

Other names:	2-Chlorobicyclo[2.2.2]octane
Inchi:	InChI=1S/C8H13Cl/c9-8-5-6-1-3-7(8)4-2-6/h6-8H,1-5H2
InchiKey:	PTVXDQZENDCNDA-UHFFFAOYSA-N
Formula:	C8H13Cl
SMILES:	ClC1CC2CCC1CC2
Mol. weight [g/mol]:	144.64
CAS:	33649-79-5

Physical Properties

Property code	Value	Unit	Source
gf	94.14	kJ/mol	Joback Method
hf	-111.25	kJ/mol	Joback Method
hfus	13.81	kJ/mol	Joback Method
hvap	37.65	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.804		Crippen Method
mcvol	114.100	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
tb	437.22	K	Joback Method
tc	654.25	K	Joback Method
tf	234.44	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.23	J/mol×K	437.22	Joback Method
cpg	249.10	J/mol×K	473.39	Joback Method
cpg	265.84	J/mol×K	509.56	Joback Method
cpg	281.49	J/mol×K	545.74	Joback Method
cpg	296.12	J/mol×K	581.91	Joback Method
cpg	309.79	J/mol×K	618.08	Joback Method
cpg	322.55	J/mol×K	654.25	Joback Method
dvisc	0.0012972	Pa×s	234.44	Joback Method

dvisc	0.0010562	Pa×s	268.24	Joback Method
dvisc	0.0009005	Pa×s	302.03	Joback Method
dvisc	0.0007927	Pa×s	335.83	Joback Method
dvisc	0.0007144	Pa×s	369.63	Joback Method
dvisc	0.0006550	Pa×s	403.42	Joback Method
dvisc	0.0006088	Pa×s	437.22	Joback Method

Sources

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=C33649795&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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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