Cyclohexane, 1-bromo-2-chloro-, cis-

Other names:	cis-1-Bromo-2-Chlorocyclohexane
	cis-2-Chlorocyclohexyl Bromide
Inchi:	InChI=1S/C6H10BrCl/c7-5-3-1-2-4-6(5)8/h5-6H,1-4H2/t5-,6+/m1/s1
InchiKey:	YUIQHWAQFBGYLI-RITPCOANSA-N
Formula:	C6H10BrCl
SMILES:	ClC1CCCCC1Br
Mol. weight [g/mol]:	197.50
CAS:	51422-75-4

Physical Properties

Property code	Value	Unit	Source
gf	18.77	kJ/mol	Joback Method
hf	-122.60	kJ/mol	Joback Method
hfus	13.68	kJ/mol	Joback Method
hvap	39.89	kJ/mol	Joback Method
ie	10.03 ± 0.02	eV	NIST Webbook
log10ws	-3.04		Crippen Method
logp	2.931		Crippen Method
mcvol	114.280	ml/mol	McGowan Method
pc	3955.54	kPa	Joback Method
tb	455.15	K	Joback Method
tc	688.23	K	Joback Method
tf	250.24	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.99	J/mol×K	455.15	Joback Method
cpg	219.48	J/mol×K	494.00	Joback Method
cpg	233.08	J/mol×K	532.84	Joback Method
cpg	245.82	J/mol×K	571.69	Joback Method
cpg	257.74	J/mol×K	610.54	Joback Method
cpg	268.85	J/mol×K	649.38	Joback Method

cpg	279.20	J/mol×K	688.23	Joback Method
dvisc	0.0035866	Pa×s	250.24	Joback Method
dvisc	0.0020086	Pa×s	284.39	Joback Method
dvisc	0.0012738	Pa×s	318.54	Joback Method
dvisc	0.0008823	Pa×s	352.69	Joback Method
dvisc	0.0006521	Pa×s	386.85	Joback Method
dvisc	0.0005061	Pa×s	421.00	Joback Method
dvisc	0.0004081	Pa×s	455.15	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=C51422754&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
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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