

Cyclohexane,1-bromo-2-chloro-,trans-

Inchi:	InChI=1S/C6H10BrCl/c7-5-3-1-2-4-6(5)8/h5-6H,1-4H2/t5-,6-/m0/s1
InchiKey:	YUIQHWAQFBGYLI-WDSKDSINSA-N
Formula:	C6H10BrCl
SMILES:	C1C1CCCCC1Br
Mol. weight [g/mol]:	197.50
CAS:	13898-96-9

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	10.13 ± 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	m ³ /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	Paxs	250.24	Joback Method

dvisc	0.0020086	Paxs	284.39	Joback Method
dvisc	0.0012738	Paxs	318.54	Joback Method
dvisc	0.0008823	Paxs	352.69	Joback Method
dvisc	0.0006521	Paxs	386.85	Joback Method
dvisc	0.0005061	Paxs	421.00	Joback Method
dvisc	0.0004081	Paxs	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=C13898969&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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