

Cyclohexane, 1-bromo-2-(trichloromethyl), trans

Inchi:	InChI=1S/C7H10BrCl3/c8-6-4-2-1-3-5(6)7(9,10)11/h5-6H,1-4H2/t5-,6-/m1/s1
InchiKey:	YHUWUUJETKWTKY-PHDIDXHHSA-N
Formula:	C7H10BrCl3
SMILES:	ClC(Cl)(Cl)C1CCCC1Br
Mol. weight [g/mol]:	280.42

Physical Properties

Property code	Value	Unit	Source
gf	6.17	kJ/mol	Joback Method
hf	-183.47	kJ/mol	Joback Method
hfus	17.25	kJ/mol	Joback Method
hvap	49.59	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.310		Crippen Method
mcvol	152.850	ml/mol	McGowan Method
pc	3299.15	kPa	Joback Method
rinpol	1488.00		NIST Webbook
tb	549.66	K	Joback Method
tc	805.47	K	Joback Method
tf	323.77	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.18	J/mol×K	549.66	Joback Method
cpg	318.96	J/mol×K	592.29	Joback Method
cpg	332.45	J/mol×K	634.93	Joback Method
cpg	344.74	J/mol×K	677.56	Joback Method
cpg	355.91	J/mol×K	720.20	Joback Method
cpg	366.04	J/mol×K	762.83	Joback Method
cpg	375.23	J/mol×K	805.47	Joback Method
dvisc	0.0036780	Pa×s	323.77	Joback Method
dvisc	0.0020052	Pa×s	361.42	Joback Method

dvisc	0.0012258	Pa×s	399.07	Joback Method
dvisc	0.0008157	Pa×s	436.71	Joback Method
dvisc	0.0005791	Pa×s	474.36	Joback Method
dvisc	0.0004323	Pa×s	512.01	Joback Method
dvisc	0.0003359	Pa×s	549.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R515276&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

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

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