

Cyclohexane, 1-chloro-2-trichloromethyl, trans

Inchi:	InChI=1S/C7H10Cl4/c8-6-4-2-1-3-5(6)7(9,10)11/h5-6H,1-4H2/t5-,6-/m1/s1
InchiKey:	SQMLDZKFEVOIOM-PHDIDXHHSA-N
Formula:	C7H10Cl4
SMILES:	C1C1CCCC1C(Cl)(Cl)Cl
Mol. weight [g/mol]:	235.97

Physical Properties

Property code	Value	Unit	Source
gf	-20.08	kJ/mol	Joback Method
hf	-225.54	kJ/mol	Joback Method
hfus	16.17	kJ/mol	Joback Method
hvap	47.54	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	4.154		Crippen Method
mvol	147.590	ml/mol	McGowan Method
pc	2931.34	kPa	Joback Method
rinpol	1436.00		NIST Webbook
tb	520.93	K	Joback Method
tc	765.68	K	Joback Method
tf	293.89	K	Joback Method
vc	0.544	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.08	J/molxK	520.93	Joback Method
cpg	307.20	J/molxK	561.72	Joback Method
cpg	321.12	J/molxK	602.51	Joback Method
cpg	333.88	J/molxK	643.30	Joback Method
cpg	345.57	J/molxK	684.10	Joback Method
cpg	356.25	J/molxK	724.89	Joback Method
cpg	365.97	J/molxK	765.68	Joback Method
dvisc	0.0047578	Paxs	293.89	Joback Method
dvisc	0.0023918	Paxs	331.73	Joback Method

dvisc	0.0013842	Paxs	369.57	Joback Method
dvisc	0.0008867	Paxs	407.41	Joback Method
dvisc	0.0006127	Paxs	445.25	Joback Method
dvisc	0.0004486	Paxs	483.09	Joback Method
dvisc	0.0003437	Paxs	520.93	Joback Method

Sources

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=R515296&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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