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: ClC1CCCCC1C(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
mcvol	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0013842	Pa×s	369.57	Joback Method
dvisc	0.0008867	Pa×s	407.41	Joback Method
dvisc	0.0006127	Pa×s	445.25	Joback Method
dvisc	0.0004486	Pa×s	483.09	Joback Method
dvisc	0.0003437	Pa×s	520.93	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=R515296&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
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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