

1-cis-2-trans-3-Trichlorocyclohexane

Inchi:	InChI=1S/C6H9Cl3/c7-4-2-1-3-5(8)6(4)9/h4-6H,1-3H2/t4-,5-/m1/s1
InchiKey:	PJBPZADYKKPBAX-RFZPGFLSSA-N
Formula:	C6H9Cl3
SMILES:	C1C1CCCC(Cl)C1Cl
Mol. weight [g/mol]:	187.50

Physical Properties

Property code	Value	Unit	Source
gf	-27.12	kJ/mol	Joback Method
hf	-200.75	kJ/mol	Joback Method
hfus	17.86	kJ/mol	Joback Method
hvap	41.92	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.993		Crippen Method
mcvol	121.260	ml/mol	McGowan Method
pc	3206.41	kPa	Joback Method
rinpol	1248.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1245.00		NIST Webbook
tb	459.18	K	Joback Method
tc	686.32	K	Joback Method
tf	246.04	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.44	J/molxK	459.18	Joback Method
cpg	283.07	J/molxK	648.47	Joback Method
cpg	272.06	J/molxK	610.61	Joback Method
cpg	260.31	J/molxK	572.75	Joback Method
cpg	247.80	J/molxK	534.89	Joback Method
cpg	234.51	J/molxK	497.04	Joback Method
cpg	293.35	J/molxK	686.32	Joback Method

dvisc	0.0003962	Paxs	459.18	Joback Method
dvisc	0.0004771	Paxs	423.66	Joback Method
dvisc	0.0005945	Paxs	388.13	Joback Method
dvisc	0.0007744	Paxs	352.61	Joback Method
dvisc	0.0010701	Paxs	317.09	Joback Method
dvisc	0.0016047	Paxs	281.56	Joback Method
dvisc	0.0027049	Paxs	246.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R591532&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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