1-cis-3-cis-5-Trichlorocyclohexane

Inchi: InChI=1S/C6H9Cl3/c7-4-1-5(8)3-6(9)2-4/h4-6H,1-3H2/t4-,5+,6-
InchiKey: VHIAVVFQACJCEC-FPFOFBBKSA-N
Formula: C6H9Cl3
SMILES: ClC1CC(Cl)CC(Cl)C1
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	1232.00		NIST Webbook
rinpol	1232.00		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/mol×K	459.18	Joback Method
cpg	283.07	J/mol×K	648.47	Joback Method
cpg	272.06	J/mol×K	610.61	Joback Method
cpg	260.31	J/mol×K	572.75	Joback Method
cpg	247.80	J/mol×K	534.89	Joback Method
cpg	234.51	J/mol×K	497.04	Joback Method
cpg	293.35	J/mol×K	686.32	Joback Method
dvisc	0.0003962	Pa×s	459.18	Joback Method

dvisc	0.0004771	Pa×s	423.66	Joback Method
dvisc	0.0005945	Pa×s	388.13	Joback Method
dvisc	0.0007744	Pa×s	352.61	Joback Method
dvisc	0.0010701	Pa×s	317.09	Joback Method
dvisc	0.0016047	Pa×s	281.56	Joback Method
dvisc	0.0027049	Pa×s	246.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R591814&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
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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