1-cis-2-trans-4-Trichlorocyclohexane

Inchi: InChI=1S/C6H9Cl3/c7-4-1-2-5(8)6(9)3-4/h4-6H,1-3H2/t4-,5-,6+/m1/s1
InchiKey: MIXOPSDQGLMAKO-PBXRRBTRSA-N
Formula: C6H9Cl3
SMILES: ClC1CCC(Cl)C(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	1261.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1258.00		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	234.51	J/mol×K	497.04	Joback Method
cpg	247.80	J/mol×K	534.89	Joback Method
cpg	260.31	J/mol×K	572.75	Joback Method

cpg	272.06	J/mol×K	610.61	Joback Method
cpg	283.07	J/mol×K	648.47	Joback Method
cpg	293.35	J/mol×K	686.32	Joback Method
dvisc	0.0027049	Pa×s	246.04	Joback Method
dvisc	0.0016047	Pa×s	281.56	Joback Method
dvisc	0.0010701	Pa×s	317.09	Joback Method
dvisc	0.0007744	Pa×s	352.61	Joback Method
dvisc	0.0005945	Pa×s	388.13	Joback Method
dvisc	0.0004771	Pa×s	423.66	Joback Method
dvisc	0.0003962	Pa×s	459.18	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=R591547&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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