1-trans-2-cis-3-cis-5-Tetrachlorocyclohexane

Inchi: InChI=1S/C6H8Cl4/c7-3-1-4(8)6(10)5(9)2-3/h3-6H,1-2H2/t3-,4+,5-,6-
InchiKey: KZUXDXMHLOTNTK-HMWJNGDSSA-N
Formula: C6H8Cl4
SMILES: ClC1CC(Cl)C(Cl)C(Cl)C1
Mol. weight [g/mol]: 221.94

Physical Properties

Property code	Value	Unit	Source
gf	-46.76	kJ/mol	Joback Method
hf	-236.83	kJ/mol	Joback Method
hfus	23.13	kJ/mol	Joback Method
hvap	45.99	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.210		Crippen Method
mcvol	133.500	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	1425.00		NIST Webbook
rinpol	1425.00		NIST Webbook
tb	491.94	K	Joback Method
tc	724.89	K	Joback Method
tf	271.72	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.99	J/mol×K	491.94	Joback Method
cpg	261.75	J/mol×K	530.76	Joback Method
cpg	274.71	J/mol×K	569.59	Joback Method
cpg	286.88	J/mol×K	608.41	Joback Method
cpg	298.26	J/mol×K	647.24	Joback Method
cpg	308.87	J/mol×K	686.06	Joback Method
cpg	318.71	J/mol×K	724.89	Joback Method
dvisc	0.0020679	Pa×s	271.72	Joback Method

dvisc	0.0013689	Pa×s	308.42	Joback Method
dvisc	0.0009893	Pa×s	345.13	Joback Method
dvisc	0.0007610	Pa×s	381.83	Joback Method
dvisc	0.0006130	Pa×s	418.53	Joback Method
dvisc	0.0005113	Pa×s	455.24	Joback Method
dvisc	0.0004381	Pa×s	491.94	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R591849&Units=SI

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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