1-Hydroxychlordene

Other names:	1,7,8,9,10,10-Hexachlorotricyclo[5.2.1.02,6]deca-4,8-dien-3-ol 3-Hydroxychlordene 4,7-Methano-1H-inden-1-ol, 4,5,6,7,8,8-hexachloro-3a,4,7,7a-tetrahydro- 4,7-Methanoinden-1-ol, 4,5,6,7,8,8-hexachloro-3a,4,7,7a-tetrahydro- Chlordene hydroxide hydroxychlordene
Inchi:	InChI=1S/C10H6Cl6O/c11-6-7(12)9(14)5-3(1-2-4(5)17)8(6,13)10(9,15)16/h1-5,17H
InchiKey:	YQWCIPIEEBVRNY-UHFFFAOYSA-N
Formula:	C10H6Cl6O
SMILES:	OC1C=CC2C1C1(Cl)C(Cl)=C(Cl)C2(Cl)C1(Cl)Cl
Mol. weight [g/mol]:	354.87
CAS:	2597-11-7

Physical Properties

Property code	Value	Unit	Source
gf	-3.87	kJ/mol	Joback Method
hf	-206.84	kJ/mol	Joback Method
hfus	29.22	kJ/mol	Joback Method
hvap	78.28	kJ/mol	Joback Method
log10ws	-5.46		Estimated Solubility Method
log10ws	-5.46		Aqueous Solubility Prediction Method
logp	3.995		Crippen Method
mcvol	189.890	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
rinpol	1955.00		NIST Webbook
rinpol	1955.00		NIST Webbook
rinpol	1955.00		NIST Webbook
tb	764.44	K	Joback Method
tc	1014.24	K	Joback Method
tf	578.64	K	Joback Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.57	J/mol×K	764.44	Joback Method
cpg	444.06	J/mol×K	806.07	Joback Method
cpg	455.80	J/mol×K	847.71	Joback Method
cpg	469.32	J/mol×K	889.34	Joback Method
cpg	485.13	J/mol×K	930.98	Joback Method
cpg	503.76	J/mol×K	972.61	Joback Method
cpg	525.74	J/mol×K	1014.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2597117&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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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