Dibenzofuran, 1,2,3,7,8,9-hexachloro

Other names: 1,2,3,7,8,9-hexachlorodibenzofuran
Inchi: InChI=1S/C12H2Cl6O/c13-3-1-5-7(11(17)9(3)15)8-6(19-5)2-4(14)10(16)12(8)18/h1-2H
InchiKey: PYUSJFJVDVSXIU-UHFFFAOYSA-N
Formula: C12H2Cl6O
SMILES: Clc1cc2oc3cc(Cl)c(Cl)c(Cl)c3c2c(Cl)c1Cl
Mol. weight [g/mol]: 374.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.92		Crippen Method
logp	7.506		Crippen Method
mcvol	200.870	ml/mol	McGowan Method
rinpol	2772.00		NIST Webbook
rinpol	2772.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R48958&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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