Dibenzofuran, 1,2,3,6,7,8-hexachloro

Other names: 1,2,3,6,7,8-hexachlorodibenzofuran
Inchi: InChI=1S/C12H2Cl6O/c13-4-1-3-7-6(2-5(14)8(15)10(7)17)19-12(3)11(18)9(4)16/h1-2H
InchiKey: JEYJJJXOFWNEHN-UHFFFAOYSA-N
Formula: C12H2Cl6O
SMILES: Clc1cc2c(oc3cc(Cl)c(Cl)c(Cl)c32)c(Cl)c1Cl
Mol. weight [g/mol]: 374.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.33		Aqueous Solubility Prediction Method
logp	7.506		Crippen Method
mcvol	200.870	ml/mol	McGowan Method
rinpol	2699.00		NIST Webbook
rinpol	2714.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R48734&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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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