1,2,3,4,7,8-Hexachlorodibenzofuran

Other names: Dibenzofuran, 1,2,3,4,7,8-hexachloro-
Inchi: InChI=1S/C12H2Cl6O/c13-4-1-3-6(2-5(4)14)19-12-7(3)8(15)9(16)10(17)11(12)18/h1-2H
InchiKey: LVYBAQIVPKCOEE-UHFFFAOYSA-N
Formula: C12H2Cl6O
SMILES: Clc1cc2oc3c(Cl)c(Cl)c(Cl)c(Cl)c3c2cc1Cl
Mol. weight [g/mol]: 374.86
CAS: 70648-26-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.66		Aqueous Solubility Prediction Method
logp	7.506		Crippen Method
mcvol	200.870	ml/mol	McGowan Method
rinpol	2693.00		NIST Webbook
rinpol	2706.00		NIST Webbook
rinpol	2708.00		NIST Webbook
rinpol	2708.00		NIST Webbook
rinpol	2693.00		NIST Webbook
rinpol	2708.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubilities of Selected PCDDs and PCDFs in Water and Various Chloride Solutions: https://www.doi.org/10.1021/je700185m
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C70648269&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