Dibenzofuran, 2,3,4,7,8-pentachloro-

Other names: 2,3,4,7,8-Pentachlorodibenzofuran
Inchi: InChI=1S/C12H3Cl5O/c13-6-1-4-5-2-8(15)10(16)11(17)12(5)18-9(4)3-7(6)14/h1-3H
InchiKey: OGBQILNBLMPPDP-UHFFFAOYSA-N
Formula: C12H3Cl5O
SMILES: Clc1cc2oc3c(Cl)c(Cl)c(Cl)cc3c2cc1Cl
Mol. weight [g/mol]: 340.42
CAS: 57117-31-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.16		Aqueous Solubility Prediction Method
logp	6.853		Crippen Method
mcvol	188.630	ml/mol	McGowan Method
rinpol	2551.00		NIST Webbook
rinpol	2536.00		NIST Webbook
rinpol	2545.00		NIST Webbook
rinpol	2551.00		NIST Webbook
rinpol	2586.00		NIST Webbook
rinpol	2586.00		NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57117314&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