Dibenzofuran, 1,2,4,7,8-pentachloro

Other names: 1,2,4,7,8-pentachlorodibenzofuran
Inchi: InChI=1S/C12H3Cl5O/c13-5-1-4-9(3-6(5)14)18-12-8(16)2-7(15)11(17)10(4)12/h1-3H
InchiKey: GCFDWHIKRXCUPJ-UHFFFAOYSA-N
Formula: C12H3Cl5O
SMILES: Clc1cc2oc3c(Cl)cc(Cl)c(Cl)c3c2cc1Cl
Mol. weight [g/mol]: 340.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.24		Crippen Method
logp	6.853		Crippen Method
mcvol	188.630	ml/mol	McGowan Method
rinpol	2505.00		NIST Webbook
rinpol	2473.00		NIST Webbook
rinpol	2505.00		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=R49085&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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