Dibenzofuran, 1,2,3,7,9-pentachloro

Other names: 1,2,3,7,9-pentachlorodibenzofuran
Inchi: InChI=1S/C12H3Cl5O/c13-4-1-5(14)9-7(2-4)18-8-3-6(15)11(16)12(17)10(8)9/h1-3H
InchiKey: JVUSEQPOWCBYNG-UHFFFAOYSA-N
Formula: C12H3Cl5O
SMILES: Clc1cc(Cl)c2c(c1)oc1cc(Cl)c(Cl)c(Cl)c12
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	2562.00		NIST Webbook
rinpol	2524.00		NIST Webbook
rinpol	2524.00		NIST Webbook

Sources

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=R48962&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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