Dibenzofuran, 1,3,4,7,8-pentachloro

Other names: 1,3,4,7,8-pentachlorodibenzofuran
Inchi: InChI=1S/C12H3Cl5O/c13-5-1-4-9(3-6(5)14)18-12-10(4)7(15)2-8(16)11(12)17/h1-3H
InchiKey: ORSUQGVCWLXKLZ-UHFFFAOYSA-N
Formula: C12H3Cl5O
SMILES: Clc1cc2oc3c(Cl)c(Cl)cc(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	2502.00		NIST Webbook
rinpol	2469.00		NIST Webbook
rinpol	2468.00		NIST Webbook
rinpol	2469.00		NIST Webbook
rinpol	2469.00		NIST Webbook
rinpol	2468.00		NIST Webbook
rinpol	2502.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R29417&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices