Dibenzofuran, 2,3,4,6,8-pentachloro

Other names: 2,3,4,6,8-pentachlorodibenzofuran
Inchi: InChI=1S/C12H3Cl5O/c13-4-1-5-6-3-7(14)9(16)10(17)12(6)18-11(5)8(15)2-4/h1-3H
InchiKey: MKRFORPSRBMAIP-UHFFFAOYSA-N
Formula: C12H3Cl5O
SMILES: Clc1cc(Cl)c2oc3c(Cl)c(Cl)c(Cl)cc3c2c1
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	2495.00		NIST Webbook
rinpol	2495.00		NIST Webbook
rinpol	2530.00		NIST Webbook
rinpol	2530.00		NIST Webbook
rinpol	2495.00		NIST Webbook
rinpol	2495.00		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=R29716&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