1,2,3,7,8-Pentachlorodibenzofuran

Other names: Dibenzofuran, 1,2,3,7,8-pentachloro-
Inchi: InChI=1S/C12H3Cl5O/c13-5-1-4-8(2-6(5)14)18-9-3-7(15)11(16)12(17)10(4)9/h1-3H
InchiKey: SBMIVUVRFPGOEB-UHFFFAOYSA-N
Formula: C12H3Cl5O
SMILES: Clc1cc2oc3cc(Cl)c(Cl)c(Cl)c3c2cc1Cl
Mol. weight [g/mol]: 340.42
CAS: 57117-41-6

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	2549.00		NIST Webbook
rinpol	2507.00		NIST Webbook
rinpol	2496.00		NIST Webbook
rinpol	2511.00		NIST Webbook
rinpol	2507.00		NIST Webbook
rinpol	2507.00		NIST Webbook
rinpol	2549.00		NIST Webbook
rinpol	2496.00		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=C57117416&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