2,3,4,6,7,8-Hexachlorodibenzofuran

Other names: Dibenzofuran, 2,3,4,6,7,8-hexachloro-
Inchi: InChI=1S/C12H2Cl6O/c13-5-1-3-4-2-6(14)8(16)10(18)12(4)19-11(3)9(17)7(5)15/h1-2H
InchiKey: XTAHLACQOVXINQ-UHFFFAOYSA-N
Formula: C12H2Cl6O
SMILES: Clc1cc2c(oc3c(Cl)c(Cl)c(Cl)cc32)c(Cl)c1Cl
Mol. weight [g/mol]: 374.86
CAS: 60851-34-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.92		Crippen Method
logp	7.506		Crippen Method
mcvol	200.870	ml/mol	McGowan Method
rinpol	2748.00		NIST Webbook
rinpol	2732.00		NIST Webbook
rinpol	2737.00		NIST Webbook
rinpol	2748.00		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=C60851345&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