Dibenzofuran, 1,2,3,4,6,8-hexachloro

Other names: 1,2,3,4,6,8-hexachlorodibenzofuran
Inchi: InChI=1S/C12H2Cl6O/c13-3-1-4-6-7(15)8(16)9(17)10(18)12(6)19-11(4)5(14)2-3/h1-2H
InchiKey: UCFGNWHERVQWMZ-UHFFFAOYSA-N
Formula: C12H2Cl6O
SMILES: Clc1cc(Cl)c2oc3c(Cl)c(Cl)c(Cl)c(Cl)c3c2c1
Mol. weight [g/mol]: 374.86

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	2650.00		NIST Webbook
rinpol	2636.00		NIST Webbook
rinpol	2656.00		NIST Webbook
rinpol	2650.00		NIST Webbook
rinpol	2636.00		NIST Webbook
rinpol	2650.00		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=R29047&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