Dibenzofuran, 1,2,7,9-tetrachloro

Other names: 1,2,7,9-tetrachlorodibenzofuran
Inchi: InChI=1S/C12H4Cl4O/c13-5-3-7(15)10-9(4-5)17-8-2-1-6(14)12(16)11(8)10/h1-4H
InchiKey: PDMFRPIFZAKMLH-UHFFFAOYSA-N
Formula: C12H4Cl4O
SMILES: Clc1cc(Cl)c2c(c1)oc1ccc(Cl)c(Cl)c12
Mol. weight [g/mol]: 305.97

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.55		Crippen Method
logp	6.200		Crippen Method
mcvol	176.390	ml/mol	McGowan Method
rinpol	2341.00		NIST Webbook
rinpol	2338.00		NIST Webbook
rinpol	2341.00		NIST Webbook
rinpol	2341.00		NIST Webbook
rinpol	2338.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R29346&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices