Dibenzofuran, 1,4,6,9-tetrachloro

Other names: 1,4,6,9-Tetrachlorodibenzofuran
Inchi: InChI=1S/C12H4Cl4O/c13-5-1-3-7(15)11-9(5)10-6(14)2-4-8(16)12(10)17-11/h1-4H
InchiKey: JAYSBJFHDJOMGZ-UHFFFAOYSA-N
Formula: C12H4Cl4O
SMILES: Clc1ccc(Cl)c2c1oc1c(Cl)ccc(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	2363.00		NIST Webbook
rinpol	2314.00		NIST Webbook
rinpol	2319.00		NIST Webbook
rinpol	2314.00		NIST Webbook
rinpol	2314.00		NIST Webbook
rinpol	2363.00		NIST Webbook
rinpol	2319.00		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=R29592&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