Dibenzofuran, 3,4,6,7-tetrachloro

Other names: 3,4,6,7-tetrachlorodibenzofuran
Inchi: InChI=1S/C12H4Cl4O/c13-7-3-1-5-6-2-4-8(14)10(16)12(6)17-11(5)9(7)15/h1-4H
InchiKey: LMJLCLBSUNZLNW-UHFFFAOYSA-N
Formula: C12H4Cl4O
SMILES: Clc1ccc2c(oc3c(Cl)c(Cl)ccc32)c1Cl
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	2362.00		NIST Webbook
rinpol	2362.00		NIST Webbook
rinpol	2353.00		NIST Webbook
rinpol	2362.00		NIST Webbook
rinpol	2353.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R29980&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