Dibenzofuran, 1,7-dichloro

Other names: 1,7-dichlorodibenzofuran
Inchi: InChI=1S/C12H6Cl2O/c13-7-4-5-8-11(6-7)15-10-3-1-2-9(14)12(8)10/h1-6H
InchiKey: XRQNHPGZRFKBJW-UHFFFAOYSA-N
Formula: C12H6Cl2O
SMILES: Clc1ccc2c(c1)oc1cccc(Cl)c12
Mol. weight [g/mol]: 237.08

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.18		Crippen Method
logp	4.893		Crippen Method
mcvol	151.910	ml/mol	McGowan Method
rinpol	1908.00		NIST Webbook
rinpol	1910.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R29663&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