Dibenzofuran, 2,7-dichloro

Other names: 2,7-dichlorodibenzofuran
Inchi: InChI=1S/C12H6Cl2O/c13-7-2-4-11-10(5-7)9-3-1-8(14)6-12(9)15-11/h1-6H
InchiKey: DOZUTNBCPVUMPY-UHFFFAOYSA-N
Formula: C12H6Cl2O
SMILES: Clc1ccc2c(c1)oc1ccc(Cl)cc12
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	1930.00		NIST Webbook
rinpol	1931.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1931.00		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=R29958&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