Dibenzofuran, 2,3,4-trichloro

Other names: 2,3,4-trichlorodibenzofuran
Inchi: InChI=1S/C12H5Cl3O/c13-8-5-7-6-3-1-2-4-9(6)16-12(7)11(15)10(8)14/h1-5H
InchiKey: YDLADWPBKZODCJ-UHFFFAOYSA-N
Formula: C12H5Cl3O
SMILES: Clc1cc2c(oc3ccccc32)c(Cl)c1Cl
Mol. weight [g/mol]: 271.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.87		Crippen Method
logp	5.546		Crippen Method
mcvol	164.150	ml/mol	McGowan Method
rinpol	2148.00		NIST Webbook
rinpol	2156.00		NIST Webbook
rinpol	2148.00		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=R29798&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

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