Dibenzofuran, 1,2,8-trichloro

Other names: 1,2,8-trichlorodibenzofuran
Inchi: InChI=1S/C12H5Cl3O/c13-6-1-3-9-7(5-6)11-10(16-9)4-2-8(14)12(11)15/h1-5H
InchiKey: UYIGPSPCOXGBCS-UHFFFAOYSA-N
Formula: C12H5Cl3O
SMILES: Clc1ccc2oc3ccc(Cl)c(Cl)c3c2c1
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	2129.00		NIST Webbook
rinpol	2121.00		NIST Webbook
rinpol	2129.00		NIST Webbook
rinpol	2129.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R29378&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices