

Dibenzofuran, 1,3,6-trichloro

Other names: 1,3,6-trichlorodibenzofuran
Inchi: InChI=1S/C12H5Cl3O/c13-6-4-9(15)11-7-2-1-3-8(14)12(7)16-10(11)5-6/h1-5H
InchiKey: AGPTXRLVBIRYLV-UHFFFAOYSA-N
Formula: C12H5Cl3O
SMILES: Clc1cc(Cl)c2c(c1)oc1c(Cl)cccc12
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	2072.00		NIST Webbook
rinpol	2071.00		NIST Webbook
rinpol	2072.00		NIST Webbook
rinpol	2071.00		NIST Webbook
rinpol	2072.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R29506&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

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