

Dibenzofuran, 1,2,3,6,7,9-hexachloro

Inchi: InChI=1S/C12H2Cl6O/c13-3-1-4(14)10(17)12-7(3)8-6(19-12)2-5(15)9(16)11(8)18/h1-2H
InchiKey: JZVOLXQREJNTTL-UHFFFAOYSA-N
Formula: C12H2Cl6O
SMILES: Clc1cc2oc3c(Cl)c(Cl)cc(Cl)c3c2c(Cl)c1Cl
Mol. weight [g/mol]: 374.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.92		Crippen Method
logp	7.506		Crippen Method
mcvol	200.870	ml/mol	McGowan Method
rinpol	2728.00		NIST Webbook

Sources

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=R48891&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/14-006-9/Dibenzofuran-1-2-3-6-7-9-hexachloro.pdf>

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