

Dibenzofuran, 1,2,3,4,8,9-hexachloro

Inchi: InChI=1S/C12H2Cl6O/c13-3-1-2-4-5(7(3)14)6-8(15)9(16)10(17)11(18)12(6)19-4/h1-2H
InchiKey: VSDUQUBUJRNREH-UHFFFAOYSA-N
Formula: C12H2Cl6O
SMILES: Clc1ccc2oc3c(Cl)c(Cl)c(Cl)c(Cl)c3c2c1Cl
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	2779.00		NIST Webbook
rinpol	2780.00		NIST Webbook
rinpol	2779.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R48720&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

Latest version available from:

<https://www.chemeo.com/cid/43-273-1/Dibenzofuran-1-2-3-4-8-9-hexachloro.pdf>

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