

Dibenzofuran, 1,2,4,6,8,9-hexachloro

Other names: 1,2,4,6,8,9-hexachlorodibenzofuran
Inchi: InChI=1S/C12H2Cl6O/c13-3-1-5(15)11-7(9(3)17)8-10(18)4(14)2-6(16)12(8)19-11/h1-2H
InchiKey: FGZCXIPKUCJGHW-UHFFFAOYSA-N
Formula: C12H2Cl6O
SMILES: Clc1cc(Cl)c2oc3c(Cl)cc(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	2686.00		NIST Webbook
rinpol	2686.00		NIST Webbook
rinpol	2685.00		NIST Webbook
rinpol	2686.00		NIST Webbook
rinpol	2685.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R29207&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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