

# Dibenzofuran, 1,3,4,8,9-pentachloro

**Inchi:** InChI=1S/C12H3Cl5O/c13-4-1-2-7-9(10(4)16)8-5(14)3-6(15)11(17)12(8)18-7/h1-3H  
**InchiKey:** QQRRQEVSMEVQB-UHFFFAOYSA-N  
**Formula:** C12H3Cl5O  
**SMILES:** Clc1cc(Cl)c2c(oc3ccc(Cl)c(Cl)c32)c1Cl  
**Mol. weight [g/mol]:** 340.42

## Physical Properties

Property code	Value	Unit	Source
log10ws	-12.24		Crippen Method
logp	6.853		Crippen Method
mcvol	188.630	ml/mol	McGowan Method
rinpole	2542.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R49320&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

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

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