

# 1,2,3,4,6-pentachlorodibenzofuran

**Other names:** Dibenzofuran, 1,2,3,4,6-pentachloro  
**Inchi:** InChI=1S/C12H3Cl5O/c13-5-3-1-2-4-6-7(14)8(15)9(16)10(17)12(6)18-11(4)5/h1-3H  
**InchiKey:** LIQJBAPSLUZUTB-UHFFFAOYSA-N  
**Formula:** C12H3Cl5O  
**SMILES:** Clc1c(Cl)c(Cl)c2c(oc3c(Cl)cccc32)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
rinpol	2496.00		NIST Webbook
rinpol	2504.00		NIST Webbook
rinpol	2496.00		NIST Webbook
rinpol	2530.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=R29051&Units=SI>

## 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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