

# 2,3,4,8,9-pentabromo-dibenzofuran

**Inchi:** InChI=1S/C12H3Br5O/c13-5-1-2-7-8(9(5)15)4-3-6(14)10(16)11(17)12(4)18-7/h1-3H  
**InchiKey:** IVBOLQBEJXWZDX-UHFFFAOYSA-N  
**Formula:** C12H3Br5O  
**SMILES:** BrC1cc2c(oc3ccc(Br)c(Br)c32)c(Br)c1Br  
**Mol. weight [g/mol]:** 562.67

## Physical Properties

Property code	Value	Unit	Source
log10ws	-14.63		Crippen Method
logp	7.398		Crippen Method
mcvol	214.930	ml/mol	McGowan Method
rinpole	3152.00		NIST Webbook
rinpole	3152.00		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=R171658&Units=SI>

## 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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