

# 1,2,3,4,6,8-hexabromo-dibenzofuran

**Inchi:** InChI=1S/C12H2Br6O/c13-3-1-4-6-7(15)8(16)9(17)10(18)12(6)19-11(4)5(14)2-3/h1-2H  
**InchiKey:** SEOUNIRJOYQFLN-UHFFFAOYSA-N  
**Formula:** C12H2Br6O  
**SMILES:** Brc1cc(Br)c2oc3c(Br)c(Br)c(Br)c(Br)c3c2c1  
**Mol. weight [g/mol]:** 641.57

## Physical Properties

Property code	Value	Unit	Source
log10ws	-15.79		Crippen Method
logp	8.161		Crippen Method
mcvol	232.430	ml/mol	McGowan Method
rinpol	3431.00		NIST Webbook
rinpol	3431.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R170422&Units=SI>  
**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>

## 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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