

# 1,2,3-tribromo-dibenzofuran

**Inchi:** InChI=1S/C12H5Br3O/c13-7-5-9-10(12(15)11(7)14)6-3-1-2-4-8(6)16-9/h1-5H  
**InchiKey:** XDHQNCQRLUFFIB-UHFFFAOYSA-N  
**Formula:** C12H5Br3O  
**SMILES:** BrC1cc2oc3ccccc3c2c(Br)c1Br  
**Mol. weight [g/mol]:** 404.88

## Physical Properties

Property code	Value	Unit	Source
log10ws	-12.30		Crippen Method
logp	5.873		Crippen Method
mcvol	179.930	ml/mol	McGowan Method
rinpol	2462.00		NIST Webbook

## Sources

**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=R170695&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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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