

# 3,6-dibromo-dibenzofuran

**Inchi:** InChI=1S/C12H6Br2O/c13-7-4-5-8-9-2-1-3-10(14)12(9)15-11(8)6-7/h1-6H  
**InchiKey:** YTPYXEPOBXHUKP-UHFFFAOYSA-N  
**Formula:** C12H6Br2O  
**SMILES:** Brc1ccc2c(c1)oc1c(Br)cccc12  
**Mol. weight [g/mol]:** 325.98

## Physical Properties

Property code	Value	Unit	Source
log10ws	-11.14		Crippen Method
logp	5.111		Crippen Method
mcvol	162.430	ml/mol	McGowan Method
rinpol	2156.00		NIST Webbook
rinpol	2156.00		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=R172097&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

Latest version available from:

<https://www.chemeo.com/cid/93-865-9/3-6-dibromo-dibenzofuran.pdf>

Generated by Cheméo on 2024-04-19 19:36:16.438160633 +0000 UTC m=+15844625.358737949.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.