# 3,4,7-tribromo-dibenzofuran

| | |
|---|---|
| **Inchi:** | InChI=1S/C12H5Br3O/c13-6-1-2-7-8-3-4-9(14)11(15)12(8)16-10(7)5-6/h1-5H |
| **InchiKey:** | PFXRHKDMKSLZHE-UHFFFAOYSA-N |
| **Formula:** | C12H5Br3O |
| **SMILES:** | Brc1ccc2c(c1)oc1c(Br)c(Br)ccc12 |
| **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 | 2491.00 | | NIST Webbook |

## Sources

| | |
|---|---|
| **Crippen Method:** | 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=R172042&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

## 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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