# 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/ci990307l |
| **Crippen Method:** | 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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