# Dibenzofuran, 1,2,3,7,8-pentabromo

**Other names:** 1,2,3,7,8-pentabromo-dibenzofuran
**Inchi:** InChI=1S/C12H3Br5O/c13-5-1-4-8(2-6(5)14)18-9-3-7(15)11(16)12(17)10(4)9/h1-3H
**InchiKey:** QMKPILUKNSMQTD-UHFFFAOYSA-N
**Formula:** C12H3Br5O
**SMILES:** Brc1cc2oc3cc(Br)c(Br)c(Br)c3c2cc1Br
**Mol. weight [g/mol]:** 562.67

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -14.63 | | Crippen Method |
| logp | 7.398 | | Crippen Method |
| mcvol | 214.930 | ml/mol | McGowan Method |
| rinpol | 3145.00 | | NIST Webbook |
| rinpol | 3177.00 | | NIST Webbook |
| rinpol | 3180.00 | | NIST Webbook |
| rinpol | 3188.00 | | NIST Webbook |
| rinpol | 3204.00 | | NIST Webbook |
| rinpol | 3204.00 | | NIST Webbook |
| rinpol | 3145.00 | | NIST Webbook |
| rinpol | 3204.00 | | NIST Webbook |
| rinpol | 3182.00 | | 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=R165985&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 |