

Dibenzofuran, 1,3,6,8-tetrachloro

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|-----------------------------|--|
| Other names: | 1,3,6,8-tetrachlorodibenzofuran |
| Inchi: | InChI=1S/C12H4Cl4O/c13-5-1-7-11-8(15)2-6(14)4-10(11)17-12(7)9(16)3-5/h1-4H |
| InchiKey: | BDXKVABZWRZKOS-UHFFFAOYSA-N |
| Formula: | C12H4Cl4O |
| SMILES: | Clc1cc(Cl)c2c(c1)oc1c(Cl)cc(Cl)cc12 |
| Mol. weight [g/mol]: | 305.97 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -11.55 | | Crippen Method |
| logp | 6.200 | | Crippen Method |
| mcvol | 176.390 | ml/mol | McGowan Method |
| rinpol | 2227.00 | | NIST Webbook |
| rinpol | 2216.00 | | NIST Webbook |
| rinpol | 2224.00 | | NIST Webbook |
| rinpol | 2227.00 | | 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=R29485&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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<https://www.cheméo.com/cid/12-185-3/Dibenzofuran-1-3-6-8-tetrachloro.pdf>

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