

Dibenzofuran, 1,2,3,6,8-pentachloro

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|-----------------------------|--|
| Inchi: | InChI=1S/C12H3Cl5O/c13-4-1-5-9-8(18-12(5)7(15)2-4)3-6(14)10(16)11(9)17/h1-3H |
| InchiKey: | VHQJZOFUPXEZQZ-UHFFFAOYSA-N |
| Formula: | C12H3Cl5O |
| SMILES: | Clc1cc(Cl)c2oc3cc(Cl)c(Cl)c(Cl)c3c2c1 |
| Mol. weight [g/mol]: | 340.42 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -12.24 | | Crippen Method |
| logp | 6.853 | | Crippen Method |
| mcvol | 188.630 | ml/mol | McGowan Method |
| rinpol | 2471.00 | | NIST Webbook |
| rinpol | 2471.00 | | 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=R48926&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 |

Latest version available from:

<https://www.chemeo.com/cid/93-857-8/Dibenzofuran-1-2-3-6-8-pentachloro.pdf>

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