

1,2,3,6,7,9-hexabromo-dibenzofuran

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|-----------------------------|--|
| Inchi: | InChI=1S/C12H2Br6O/c13-3-1-4(14)10(17)12-7(3)8-6(19-12)2-5(15)9(16)11(8)18/h1-2H |
| InchiKey: | YZRKGWPYPQWZHK-UHFFFAOYSA-N |
| Formula: | C12H2Br6O |
| SMILES: | BrC1cc2oc3c(Br)c(Br)cc(Br)c3c2c(Br)c1Br |
| 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 |
| rinpole | 3521.00 | | 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=R170551&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| rinpole: | Non-polar retention indices |

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