

2,3,4,8-tetrabromo-dibenzofuran

Inchi: InChI=1S/C12H4Br4O/c13-5-1-2-9-6(3-5)7-4-8(14)10(15)11(16)12(7)17-9/h1-4H
InchiKey: UPTXKXSOCQVGFU-UHFFFAOYSA-N
Formula: C12H4Br4O
SMILES: BrC1ccc2oc3c(Br)c(Br)c(Br)cc3c2c1
Mol. weight [g/mol]: 483.78

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -13.47 | | Crippen Method |
| logp | 6.636 | | Crippen Method |
| mcvol | 197.430 | ml/mol | McGowan Method |
| rinpola | 2816.00 | | 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=R171663&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
rinpola: Non-polar retention indices

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<https://www.chemeo.com/cid/35-430-5/2-3-4-8-tetrabromo-dibenzofuran.pdf>

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