

Dibenzofuran, 2,3,7,8-tetrabromo-

Other names: 2,3,7,8-Tetrabromodibenzofuran
Inchi: InChI=1S/C12H4Br4O/c13-7-1-5-6-2-8(14)10(16)4-12(6)17-11(5)3-9(7)15/h1-4H
InchiKey: HCSR VQXNLHZQNM-UHFFFAOYSA-N
Formula: C12H4Br4O
SMILES: BrC1cc2oc3cc(Br)c(Br)cc3c2cc1Br
Mol. weight [g/mol]: 483.78
CAS: 67733-57-7

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -13.47 | | Crippen Method |
| logp | 6.636 | | Crippen Method |
| mcvol | 197.430 | ml/mol | McGowan Method |
| rinpol | 2816.00 | | NIST Webbook |
| rinpol | 2847.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C67733577&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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