

Dibenzofuran, 3,4,6,7-tetrachloro

Other names: 3,4,6,7-tetrachlorodibenzofuran
Inchi: InChI=1S/C12H4Cl4O/c13-7-3-1-5-6-2-4-8(14)10(16)12(6)17-11(5)9(7)15/h1-4H
InchiKey: LMJLCLBSUNZLNW-UHFFFAOYSA-N
Formula: C12H4Cl4O
SMILES: Clc1ccc2c(oc3c(Cl)c(Cl)ccc32)c1Cl
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 | 2362.00 | | NIST Webbook |
| rinpol | 2362.00 | | NIST Webbook |
| rinpol | 2353.00 | | NIST Webbook |
| rinpol | 2362.00 | | NIST Webbook |
| rinpol | 2353.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R29980&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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