

Dibenzofuran, 1,2,6-trichloro

Other names: 1,2,6-trichlorodibenzofuran
Inchi: InChI=1S/C12H5Cl3O/c13-7-4-5-9-10(11(7)15)6-2-1-3-8(14)12(6)16-9/h1-5H
InchiKey: CYRZCBUWRUACKJ-UHFFFAOYSA-N
Formula: C12H5Cl3O
SMILES: Clc1ccc2oc3c(Cl)cccc3c2c1Cl
Mol. weight [g/mol]: 271.53

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -10.87 | | Crippen Method |
| logp | 5.546 | | Crippen Method |
| mcvol | 164.150 | ml/mol | McGowan Method |
| rinpol | 2125.00 | | NIST Webbook |
| rinpol | 2132.00 | | NIST Webbook |
| rinpol | 2125.00 | | NIST Webbook |
| rinpol | 2132.00 | | NIST Webbook |

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R29328&Units=SI>

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/15-807-9/Dibenzofuran-1-2-6-trichloro.pdf>

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