

# Dibenzofuran, 1,2,3,6-tetrachloro

|                             |                                                                           |
|-----------------------------|---------------------------------------------------------------------------|
| <b>Other names:</b>         | 1,2,3,6-tetrachlorodibenzofuran                                           |
| <b>Inchi:</b>               | InChI=1S/C12H4Cl4O/c13-6-3-1-2-5-9-8(17-12(5)6)4-7(14)10(15)11(9)16/h1-4H |
| <b>InchiKey:</b>            | BBAXFLIBRPXRBP-UHFFFAOYSA-N                                               |
| <b>Formula:</b>             | C12H4Cl4O                                                                 |
| <b>SMILES:</b>              | Clc1cc2oc3c(Cl)cccc3c2c(Cl)c1Cl                                           |
| <b>Mol. weight [g/mol]:</b> | 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        | 2307.00 |        | NIST Webbook   |
| rinpol        | 2318.00 |        | NIST Webbook   |
| rinpol        | 2307.00 |        | NIST Webbook   |
| rinpol        | 2318.00 |        | NIST Webbook   |

## Sources

|                        |                                                                                                                                         |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                               |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                       |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                   |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R29136&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R29136&amp;Units=SI</a> |

## Legend

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

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