

# Dibenzofuran, 1,2,3,8-tetrachloro

|                      |                                                                            |
|----------------------|----------------------------------------------------------------------------|
| Other names:         | 1,2,3,8-Tetrachlorodibenzofuran                                            |
| Inchi:               | InChI=1S/C12H4Cl4O/c13-5-1-2-8-6(3-5)10-9(17-8)4-7(14)11(15)12(10)16/h1-4H |
| InchiKey:            | KFQRHGKKSHJMCO-UHFFFAOYSA-N                                                |
| Formula:             | C12H4Cl4O                                                                  |
| SMILES:              | Clc1ccc2oc3cc(Cl)c(Cl)c(Cl)c3c2c1                                          |
| 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        | 2308.00 |        | NIST Webbook   |
| rinpol        | 2307.00 |        | NIST Webbook   |
| rinpol        | 2307.00 |        | NIST Webbook   |
| rinpol        | 2307.00 |        | NIST Webbook   |

## Sources

|                 |                                                                                                                                         |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                   |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R29168&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R29168&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                               |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                       |

## 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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