

Dibenzofuran, 1,2,4,6-tetrachloro

Other names: 1,2,4,6-Tetrachlorodibenzofuran
Inchi: InChI=1S/C12H4Cl4O/c13-6-3-1-2-5-9-10(16)7(14)4-8(15)12(9)17-11(5)6/h1-4H
InchiKey: NLVWEKPFUPVMZ-UHFFFAOYSA-N
Formula: C12H4Cl4O
SMILES: Clc1cc(Cl)c2oc3c(Cl)cccc3c2c1Cl
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	2270.00		NIST Webbook
rinpol	2264.00		NIST Webbook
rinpol	2264.00		NIST Webbook
rinpol	2264.00		NIST Webbook

Sources

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=R29225&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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/11-952-2/Dibenzofuran-1-2-4-6-tetrachloro.pdf>

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