

6-methyl-2,3,4,8-tetrachlorodibenzofuran

Inchi: InChI=1S/C13H6Cl4O/c1-5-2-6(14)3-7-8-4-9(15)10(16)11(17)13(8)18-12(5)7/h2-4H,1H3
InchiKey: OIWCQHWPBWRPQBC-UHFFFAOYSA-N
Formula: C13H6Cl4O
SMILES: Cc1cc(Cl)cc2c1oc1c(Cl)c(Cl)c(Cl)cc12
Mol. weight [g/mol]: 320.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.03		Crippen Method
logp	6.508		Crippen Method
mcvol	190.480	ml/mol	McGowan Method
rinpol	2419.00		NIST Webbook
rinpol	2419.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R173416&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

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