

2,3,4,9-tetrabromo-dibenzofuran

Inchi: InChI=1S/C12H4Br4O/c13-6-2-1-3-8-9(6)5-4-7(14)10(15)11(16)12(5)17-8/h1-4H
InchiKey: HDFZMRCHMSCVMH-UHFFFAOYSA-N
Formula: C12H4Br4O
SMILES: BrC1cc2c(oc3cccc(Br)c32)c(Br)c1Br
Mol. weight [g/mol]: 483.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.47		Crippen Method
logp	6.636		Crippen Method
mcvol	197.430	ml/mol	McGowan Method
rinpol	2792.00		NIST Webbook
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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=R171678&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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