

1,2,4,9-tetrabromo-dibenzofuran

Inchi: InChI=1S/C12H4Br4O/c13-5-2-1-3-8-9(5)10-11(16)6(14)4-7(15)12(10)17-8/h1-4H
InchiKey: IMSGIHSYTWQBIP-UHFFFAOYSA-N
Formula: C12H4Br4O
SMILES: Brc1cc(Br)c2oc3cccc(Br)c3c2c1Br
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	2813.00		NIST Webbook
rinpol	2813.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=R170808&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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<https://www.chemeo.com/cid/17-261-3/1-2-4-9-tetrabromo-dibenzofuran.pdf>

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