

1,4,9-tribromo-dibenzofuran

Inchi: InChI=1S/C12H5Br3O/c13-6-2-1-3-9-10(6)11-7(14)4-5-8(15)12(11)16-9/h1-5H
InchiKey: SOBCQEWGYN AZQC-UHFFFAOYSA-N
Formula: C12H5Br3O
SMILES: BrC1ccc(Br)c2c1oc1cccc(Br)c12
Mol. weight [g/mol]: 404.88

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.30		Crippen Method
logp	5.873		Crippen Method
mcvol	179.930	ml/mol	McGowan Method
rinpol	2491.00		NIST Webbook
rinpol	2491.00		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=R171405&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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