

1,3,6,7-tetrabromo-dibenzofuran

Inchi: InChI=1S/C12H4Br4O/c13-5-3-8(15)10-6-1-2-7(14)11(16)12(6)17-9(10)4-5/h1-4H
InchiKey: HJAHYZGENLXMRX-UHFFFAOYSA-N
Formula: C12H4Br4O
SMILES: BrC1cc(Br)c2c(c1)oc1c(Br)c(Br)ccc12
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	2739.00		NIST Webbook
rinpol	2739.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R171123&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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