

1,4-dibromo-dibenzofuran

Inchi: InChI=1S/C12H6Br2O/c13-8-5-6-9(14)12-11(8)7-3-1-2-4-10(7)15-12/h1-6H
InchiKey: SJPWYOJYEGIRLP-UHFFFAOYSA-N
Formula: C12H6Br2O
SMILES: Brc1ccc(Br)c2c1oc1ccccc12
Mol. weight [g/mol]: 325.98

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.14		Crippen Method
logp	5.111		Crippen Method
mcvol	162.430	ml/mol	McGowan Method
rinpol	2122.00		NIST Webbook
rinpol	2122.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R171425&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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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