

3,4-dibromo-dibenzofuran

Inchi: InChI=1S/C12H6Br2O/c13-9-6-5-8-7-3-1-2-4-10(7)15-12(8)11(9)14/h1-6H
InchiKey: PSQANSIANLLSPC-UHFFFAOYSA-N
Formula: C12H6Br2O
SMILES: Brc1ccc2c(oc3ccccc32)c1Br
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	2176.00		NIST Webbook
rinpol	2176.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R172077&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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/93-864-0/3-4-dibromo-dibenzofuran.pdf>

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