

1,8-dibromo-dibenzofuran

Inchi:	InChI=1S/C12H6Br2O/c13-7-4-5-10-8(6-7)12-9(14)2-1-3-11(12)15-10/h1-6H
InchiKey:	VCIOALQVPMTGGE-UHFFFAOYSA-N
Formula:	C12H6Br2O
SMILES:	BrC1ccc2oc3cccc(Br)c3c2c1
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	2130.00		NIST Webbook
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Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R171485&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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