

2,3-dibromo-dibenzofuran

Inchi:	InChI=1S/C12H6Br2O/c13-9-5-8-7-3-1-2-4-11(7)15-12(8)6-10(9)14/h1-6H
InchiKey:	SNOGWHFJQWWBDP-UHFFFAOYSA-N
Formula:	C12H6Br2O
SMILES:	BrC1cc2oc3ccccc3c2cc1Br
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	2150.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R171836&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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