

3-bromo-dibenzofuran

Inchi:	InChI=1S/C12H7BrO/c13-8-5-6-10-9-3-1-2-4-11(9)14-12(10)7-8/h1-7H
InchiKey:	AZFABGHLDGJASW-UHFFFAOYSA-N
Formula:	C12H7BrO
SMILES:	BrC1ccc2c(c1)oc1ccccc12
Mol. weight [g/mol]:	247.09

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.98		Crippen Method
logp	4.348		Crippen Method
mcvol	144.930	ml/mol	McGowan Method
rinpola	1849.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R172166&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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<https://www.chemeo.com/cid/93-912-6/3-bromo-dibenzofuran.pdf>

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