

# 3,4,6-tribromo-dibenzofuran

<b>Inchi:</b>	InChI=1S/C12H5Br3O/c13-8-5-4-7-6-2-1-3-9(14)11(6)16-12(7)10(8)15/h1-5H
<b>InchiKey:</b>	HVBWHLFLULUOHT-UHFFFAOYSA-N
<b>Formula:</b>	C12H5Br3O
<b>SMILES:</b>	BrC1ccc2c(oc3c(Br)cccc32)c1Br
<b>Mol. weight [g/mol]:</b>	404.88

## Physical Properties

Property code	Value	Unit	Source
log10ws	-12.30		Crippen Method
logp	5.873		Crippen Method
mcvol	179.930	ml/mol	McGowan Method
rinpol	2491.00		NIST Webbook

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R172037&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R172037&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

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

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