

# 1,3,4,7,9-pentabromo-dibenzofuran

<b>Inchi:</b>	InChI=1S/C12H3Br5O/c13-4-1-5(14)9-8(2-4)18-12-10(9)6(15)3-7(16)11(12)17/h1-3H
<b>InchiKey:</b>	HRCFIJWEFSMLEC-UHFFFAOYSA-N
<b>Formula:</b>	C12H3Br5O
<b>SMILES:</b>	BrC1cc(Br)c2c(c1)oc1c(Br)c(Br)cc(Br)c12
<b>Mol. weight [g/mol]:</b>	562.67

## Physical Properties

Property code	Value	Unit	Source
log10ws	-14.63		Crippen Method
logp	7.398		Crippen Method
mcvol	214.930	ml/mol	McGowan Method
rinpol	3098.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<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=R171069&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R171069&amp;Units=SI</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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