

# 1,2,3,6,7-pentabromo-dibenzofuran

<b>Inchi:</b>	InChI=1S/C12H3Br5O/c13-5-2-1-4-8-7(18-12(4)10(5)16)3-6(14)9(15)11(8)17/h1-3H
<b>InchiKey:</b>	OYKGVILGNBNCKY-UHFFFAOYSA-N
<b>Formula:</b>	C12H3Br5O
<b>SMILES:</b>	BrC1cc2oc3c(Br)c(Br)ccc3c2c(Br)c1Br
<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	3164.00		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=R170566&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R170566&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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