

# 2-Bromodibenzofuran

<b>Inchi:</b>	InChI=1S/C12H7BrO/c13-8-5-6-12-10(7-8)9-3-1-2-4-11(9)14-12/h1-7H
<b>InchiKey:</b>	CRJISNQTZDMKQD-UHFFFAOYSA-N
<b>Formula:</b>	C12H7BrO
<b>SMILES:</b>	Brc1ccc2oc3ccccc3c2c1
<b>Mol. weight [g/mol]:</b>	247.09
<b>CAS:</b>	86-76-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-9.98		Crippen Method
logp	4.348		Crippen Method
mcvol	144.930	ml/mol	McGowan Method
rinpol	1851.00		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=C86760&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C86760&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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