

# Broxaldine

<b>Other names:</b>	8-Quinolinol, 5,7-dibromo-2-methyl-, benzoate 5,7-Dibromo-2-methyl-8-quinolinol benzoate ester Brobenzoxaldine 5,7-Dibrom-2-methyl-8-chinolyl benzoat 5,7-Dibromo-8-benzoyloxyquinaldine
<b>Inchi:</b>	InChI=1S/C17H11Br2NO2/c1-10-7-8-12-13(18)9-14(19)16(15(12)20-10)22-17(21)11-5-3
<b>InchiKey:</b>	IJTPLVAAROHGGB-UHFFFAOYSA-N
<b>Formula:</b>	C17H11Br2NO2
<b>SMILES:</b>	Cc1ccc2c(Br)cc(Br)c(OC(=O)c3ccccc3)c2n1
<b>Mol. weight [g/mol]:</b>	421.08
<b>CAS:</b>	3684-46-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.93		Crippen Method
logp	5.287		Crippen Method
mcvol	235.830	ml/mol	McGowan Method
rinpol	2686.00		NIST Webbook
rinpol	2686.00		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=C3684466&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3684466&amp;Units=SI</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

**rinpol:** Non-polar retention indices

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