Broxaldine

Other names:	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
Inchi:	InChI=1S/C17H11Br2NO2/c1-10-7-8-12-13(18)9-14(19)16(15(12)20-10)22-17(21)11-5-3-
InchiKey:	IJTPLVAAROHGGB-UHFFFAOYSA-N
Formula:	C17H11Br2NO2
SMILES:	Cc1ccc2c(Br)cc(Br)c(OC(=O)c3ccccc3)c2n1
Mol. weight [g/mol]:	421.08
CAS:	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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3684466&Units=SI

Legend

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

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices