

Benoxacor

Other names:	Ethanone, 2,2-dichloro-1-(2,3-dihydro-3-methyl-4H-1,4-benzoxazin-4-yl)-
Inchi:	InChI=1S/C11H11Cl2NO2/c1-7-6-16-9-5-3-2-4-8(9)14(7)11(15)10(12)13/h2-5,7,10H,6H2
InchiKey:	PFJJMJDEVLPNE-UHFFFAOYSA-N
Formula:	C11H11Cl2NO2
SMILES:	CC1COc2ccccc2N1C(=O)C(Cl)Cl
Mol. weight [g/mol]:	260.12
CAS:	98730-04-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.03		Crippen Method
logp	2.604		Crippen Method
mcvol	173.130	ml/mol	McGowan Method
rinpola	1853.00		NIST Webbook
rinpola	1853.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98730042&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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<https://www.chemeo.com/cid/61-430-6/Benoxacor.pdf>

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