

8-Hydroxynorloxapine

Other names:	8-Hydroxyamoxapine
Inchi:	InChI=1S/C17H16ClN3O2/c18-11-1-3-15-13(9-11)17(21-7-5-19-6-8-21)20-14-10-12(22)2
InchiKey:	QDWNOKXUZTYVGO-UHFFFAOYSA-N
Formula:	C17H16ClN3O2
SMILES:	<chem>Oc1ccc2c(c1)N=C(N1CCNCC1)c1cc(Cl)ccc1O2</chem>
Mol. weight [g/mol]:	329.78
CAS:	61443-78-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.27		Crippen Method
logp	3.135		Crippen Method
mcvol	230.770	ml/mol	McGowan Method
rmpol	2907.00		NIST Webbook
rmpol	2907.00		NIST Webbook

Sources

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=C61443785&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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