

Viloxazine, N-acetyl-

Other names:	Viloxazine, acetylated
Inchi:	InChI=1S/C15H21NO4/c1-3-18-14-6-4-5-7-15(14)20-11-13-10-16(12(2)17)8-9-19-13/h4-
InchiKey:	BVUHTRYNQIXGLZ-UHFFFAOYSA-N
Formula:	C15H21NO4
SMILES:	CCOc1cccc1OCC1CN(C(C)=O)CCO1
Mol. weight [g/mol]:	279.33
CAS:	33585-04-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.08		Crippen Method
logp	1.711		Crippen Method
mcvol	216.750	ml/mol	McGowan Method
rinsol	2219.00		NIST Webbook
rinsol	2219.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33585045&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
rinsol:	Non-polar retention indices

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