

Viloxazine M(HO), acetylated

Inchi: InChI=1S/C17H23NO6/c1-4-21-17-9-14(24-13(3)20)5-6-16(17)23-11-15-10-18(12(2)19)7
InchiKey: HSEMWPGRGUDTAI-UHFFFAOYSA-N
Formula: C17H23NO6
SMILES: CCOc1cc(OC(C)=O)ccc1OCC1CN(C(C)=O)CCO1
Mol. weight [g/mol]: 337.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	1.637		Crippen Method
mcvol	252.370	ml/mol	McGowan Method
rinpol	2610.00		NIST Webbook
rinpol	2610.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R311272&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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
rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/64-690-5/Viloxazine-M-HO-acetylated.pdf>

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