

Oxomemazine M (bis-nor-), acetylated

Inchi: InChI=1S/C18H20N2O3S/c1-13(11-19-14(2)21)12-20-15-7-3-5-9-17(15)24(22,23)18-10-6
InchiKey: IBELYQOZAPJGES-UHFFFAOYSA-N
Formula: C18H20N2O3S
SMILES: CC(=O)NCC(C)CN1c2ccccc2S(=O)(=O)c2ccccc21
Mol. weight [g/mol]: 344.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.60		Crippen Method
logp	2.743		Crippen Method
mcvol	255.720	ml/mol	McGowan Method
rinsol	3035.00		NIST Webbook
rinsol	3035.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R314459&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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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