

Alimemazine M (nor-), monoacetylated

Other names: Alimemazine M (nor-), acetylated
Inchi: InChI=1S/C19H22N2OS/c1-14(12-20(3)15(2)22)13-21-16-8-4-6-10-18(16)23-19-11-7-5-9
InchiKey: WKCMHDURNBYVKR-UHFFFAOYSA-N
Formula: C19H22N2OS
SMILES: CC(=O)N(C)CC(C)CN1c2ccccc2Sc2ccccc21
Mol. weight [g/mol]: 326.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.45		Crippen Method
logp	4.404		Crippen Method
mcvol	258.070	ml/mol	McGowan Method
rinpol	2710.00		NIST Webbook
rinpol	2709.00		NIST Webbook
rinpol	2710.00		NIST Webbook
rinpol	2709.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R310140&Units=SI>

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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