Alimemazine M (bis-nor-), monoacetylated

Other names: Alimemazine M (bis-nor-), acetylated
Inchi: InChI=1S/C18H20N2OS/c1-13(11-19-14(2)21)12-20-15-7-3-5-9-17(15)22-18-10-6-4-8-16
InchiKey: KTURKTZAIPJFPF-UHFFFAOYSA-N
Formula: C18H20N2OS
SMILES: CC(=O)NCC(C)CN1c2ccccc2Sc2ccccc21
Mol. weight [g/mol]: 312.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.65		Crippen Method
logp	4.061		Crippen Method
mcvol	243.980	ml/mol	McGowan Method
rinpol	2765.00		NIST Webbook
rinpol	2767.00		NIST Webbook
rinpol	2767.00		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=R310120&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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