Alimemazine M (nor-HO-), diacetylated

Other names: Alimemazine M (nor-hydroxy-), acetylated
Inchi: InChI=1S/C21H24N2O3S/c1-14(12-22(4)15(2)24)13-23-18-7-5-6-8-20(18)27-21-11-17(2
InchiKey: NZWAAAOIILAEPO-UHFFFAOYSA-N
Formula: C21H24N2O3S
SMILES: CC(=O)Oc1ccc2c(c1)Sc1ccccc1N2CC(C)CN(C)C(C)=O
Mol. weight [g/mol]: 384.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.77		Crippen Method
logp	4.329		Crippen Method
mcvol	293.690	ml/mol	McGowan Method
rinpol	2930.00		NIST Webbook
rinpol	2930.00		NIST Webbook
rinpol	2930.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R310155&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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