

Alimemazine M (HO-), acetylated

Other names: Alimemazine M (hydroxy-), acetylated
Inchi: InChI=1S/C20H24N2O2S/c1-14(12-21(3)4)13-22-17-7-5-6-8-19(17)25-20-11-16(24-15(2
InchiKey: ZQAKZDUDVCBPBB-UHFFFAOYSA-N
Formula: C20H24N2O2S
SMILES: CC(=O)Oc1ccc2c(c1)Sc1cccc1N2CC(C)CN(C)C
Mol. weight [g/mol]: 356.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.57		Crippen Method
logp	4.412		Crippen Method
mcvol	278.030	ml/mol	McGowan Method
rinpol	2600.00		NIST Webbook
rinpol	2550.00		NIST Webbook
rinpol	2600.00		NIST Webbook
rinpol	2600.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R310135&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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