

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/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/38-552-7/Alimemazine-M-bis-nor-monoacetylated.pdf>

Generated by Cheméo on 2024-04-26 20:52:30.799865064 +0000 UTC m=+16453999.720442381.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.