Prothipendyl M (nor-), acetylated

Inchi: InChI=1S/C17H19N3OS/c1-13(21)19(2)11-6-12-20-14-7-3-4-8-15(14)22-16-9-5-10-18-17

InchiKey: NSXBJZTYHWVUPP-UHFFFAOYSA-N

Formula: C17H19N3OS

SMILES: CC(=O)N(C)CCCN1c2ccccc2Sc2cccnc21

Mol. weight [g/mol]: 313.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.04		Crippen Method
logp	3.553		Crippen Method
mcvol	239.870	ml/mol	McGowan Method
rinpol	2880.00		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=R310620&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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