

Isothipendyl M (nor-), acetylated

Inchi: InChI=1S/C17H19N3OS/c1-12(19(3)13(2)21)11-20-14-7-4-5-8-15(14)22-16-9-6-10-18-17
InchiKey: REHPXIVERWVYDK-UHFFFAOYSA-N
Formula: C17H19N3OS
SMILES: CC(=O)N(C)C(C)CN1c2ccccc2Sc2cccnc21
Mol. weight [g/mol]: 313.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.15		Crippen Method
logp	3.551		Crippen Method
mcvol	239.870	ml/mol	McGowan Method
rinpole	2600.00		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=R314375&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
rinpole: Non-polar retention indices

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<https://www.chemeo.com/cid/22-572-2/Isothipendyl-M-nor-acetylated.pdf>

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