

Isothipendyl M (bis-nor-), acetylated

Inchi: InChI=1S/C16H17N3OS/c1-11(18-12(2)20)10-19-13-6-3-4-7-14(13)21-15-8-5-9-17-16(15)
InchiKey: XASMCFUUVQVGXLB-UHFFFAOYSA-N
Formula: C16H17N3OS
SMILES: CC(=O)NC(C)CN1c2ccccc2Sc2cccnc21
Mol. weight [g/mol]: 299.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.35		Crippen Method
logp	3.209		Crippen Method
mcvol	225.780	ml/mol	McGowan Method
rinpole	2520.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R314340&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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