Prothipendyl M (bis-nor-), monoacetylated

Inchi: InChI=1S/C16H17N3OS/c1-12(20)17-10-5-11-19-13-6-2-3-7-14(13)21-15-8-4-9-18-16(15
InchiKey: DFWHWRXTYVGKHM-UHFFFAOYSA-N
Formula: C16H17N3OS
SMILES: CC(=O)NCCCN1c2ccccc2Sc2cccnc21
Mol. weight [g/mol]: 299.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.24		Crippen Method
logp	3.211		Crippen Method
mcvol	225.780	ml/mol	McGowan Method
rinpol	2830.00		NIST Webbook
rinpol	2830.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R310600&Units=SI

Legend

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

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