Prothipendyl M (nor-HO-), diacetylated

Inchi: InChI=1S/C20H22N2O3S/c1-14(23)21(3)11-6-12-22-17-7-4-5-8-19(17)26-20-13-16(25-15

InchiKey: LTQJFGVIAUHUJW-UHFFFAOYSA-N

Formula: C20H22N2O3S

SMILES: CC(=O)Oc1ccc2c(c1)Sc1ccccc1N2CCCN(C)C(C)=O

Mol. weight [g/mol]: 370.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.59		Crippen Method
logp	4.083		Crippen Method
mcvol	279.600	ml/mol	McGowan Method
rinpol	3070.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310635&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices