

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(25-1
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

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<https://www.chemeo.com/cid/47-459-1/Prothipendyl-M-nor-HO-diacetylated.pdf>

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