Isothipendyl M (hydroxy-), acetylated

Inchi: InChI=1S/C18H21N3O2S/c1-12(20(3)4)11-21-15-8-7-14(23-13(2)22)10-17(15)24-16-6-5-
InchiKey: CWBFQGTZPJAVEO-UHFFFAOYSA-N
Formula: C18H21N3O2S
SMILES: CC(=O)Oc1ccc2c(c1)Sc1cccnc1N2CC(C)N(C)C
Mol. weight [g/mol]: 343.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.27		Crippen Method
logp	3.560		Crippen Method
mcvol	259.830	ml/mol	McGowan Method
rinpol	2640.00		NIST Webbook
rinpol	2640.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R314355&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.