

# Isothipendyl M (nor-hydroxy-), acetylated

**Inchi:** InChI=1S/C19H21N3O3S/c1-12(21(4)13(2)23)11-22-16-8-7-15(25-14(3)24)10-18(16)26-  
**InchiKey:** UVYHWCWLXCOADB-UHFFFAOYSA-N  
**Formula:** C19H21N3O3S  
**SMILES:** CC(=O)Oc1ccc2c(c1)Sc1cccnc1N2CC(C)N(C)C(C)=O  
**Mol. weight [g/mol]:** 371.45

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.47		Crippen Method
logp	3.476		Crippen Method
mcvol	275.490	ml/mol	McGowan Method
rinpole	2940.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R314380&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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  
**rinpole:** Non-polar retention indices

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