

# Isothipendyl M (hydroxy-ring), acetylated

**Inchi:** InChI=1S/C15H12N2O3S/c1-9(18)17-12-6-5-11(20-10(2)19)8-14(12)21-13-4-3-7-16-15(17)  
**InchiKey:** MFNCZKQVIFYRPGB-UHFFFAOYSA-N  
**Formula:** C15H12N2O3S  
**SMILES:** CC(=O)Oc1ccc2c(c1)Sc1cccnc1N2C(C)=O  
**Mol. weight [g/mol]:** 300.33

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.11		Crippen Method
logp	3.156		Crippen Method
mcvol	209.150	ml/mol	McGowan Method
rinpola	2575.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=R314360&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/32-517-2/Isothipendyl-M-hydroxy-ring-acetylated.pdf>

Generated by Cheméo on 2024-04-30 15:52:23.612848363 +0000 UTC m=+16781592.533425675.

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