# 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(1
**InchiKey:** MFNCZKQVFYRPGB-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 |
| rinpol | 2575.00 | | NIST Webbook |

## Sources

**Crippen Method:** 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
**rinpol:** Non-polar retention indices