

# Promethazine M (HO-), monoacetylated

**Other names:** Promethazine M (hydroxy-), acetylated  
**Inchi:** InChI=1S/C19H22N2O2S/c1-13(20(3)4)12-21-16-7-5-6-8-18(16)24-19-11-15(23-14(2)22  
**InchiKey:** RUHZYJBTFIIOKB-UHFFFAOYSA-N  
**Formula:** C19H22N2O2S  
**SMILES:** CC(=O)Oc1ccc2c(c1)Sc1cccc1N2CC(C)N(C)C  
**Mol. weight [g/mol]:** 342.45

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -4.51   |        | Crippen Method |
| logp          | 4.165   |        | Crippen Method |
| mcvol         | 263.940 | ml/mol | McGowan Method |
| rinpol        | 2690.00 |        | NIST Webbook   |
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| rinpol        | 2690.00 |        | NIST Webbook   |

## Sources

**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)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R310571&Units=SI>

## 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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