# Acepromethazine M (dihydro-), monoacetylated

**Inchi:** InChI=1S/C22H28N2O2S/c1-15(13-23(4)5)14-24-19-8-6-7-9-21(19)27-22-11-10-18(12-2

**InchiKey:** LARJGEAEJXHGKH-UHFFFAOYSA-N

**Formula:** C22H28N2O2S

**SMILES:** CC(=O)OC(C)c1ccc2c(c1)N(CC(C)CN(C)C)c1ccccc1S2

**Mol. weight [g/mol]:** 384.54

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -5.22 | | Crippen Method |
| logp | 5.111 | | Crippen Method |
| mcvol | 306.210 | ml/mol | McGowan Method |
| rinpol | 2690.00 | | NIST Webbook |

## Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R310091&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