

# Mequitazine M (hydroxy-ring), acetylated

**Inchi:** InChI=1S/C22H24N2O2S/c1-15(25)26-18-6-7-20-22(12-18)27-21-5-3-2-4-19(21)24(20)1  
**InchiKey:** PVFNARVJNNWVFE-UHFFFAOYSA-N  
**Formula:** C22H24N2O2S  
**SMILES:** CC(=O)Oc1ccc2c(c1)Sc1cccc1N2CC1CN2CCC1CC2  
**Mol. weight [g/mol]:** 380.50

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.96		Crippen Method
logp	4.556		Crippen Method
mcvol	284.490	ml/mol	McGowan Method
rinpole	2550.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R314404&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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>

## 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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