

# Perphenazine M (desalkyl-), acetylated

**Inchi:** InChI=1S/C21H24ClN3OS/c1-16(26)24-13-11-23(12-14-24)9-4-10-25-18-5-2-3-6-20(18)2  
**InchiKey:** KLNDQNASBQSBEA-UHFFFAOYSA-N  
**Formula:** C21H24ClN3OS  
**SMILES:** CC(=O)N1CCN(CCCN2c3ccccc3Sc3ccc(Cl)cc32)CC1  
**Mol. weight [g/mol]:** 401.95

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.68		Crippen Method
logp	4.497		Crippen Method
mcvol	297.610	ml/mol	McGowan Method
rinpol	3500.00		NIST Webbook
rinpol	3500.00		NIST Webbook
rinpol	3500.00		NIST Webbook
rinpol	3500.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R310506&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  
**rinpol:** Non-polar retention indices

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