

# 2-Acetyl-1,2,3,4,9,13b-hexahydro-2,4a-diaza-triben

**Other names:** Mianserin M(Nor), acetylated  
**Inchi:** InChI=1S/C19H20N2O/c1-14(22)20-10-11-21-18-9-5-3-7-16(18)12-15-6-2-4-8-17(15)19(20)  
**InchiKey:** KLGVRKZVHNSAFM-UHFFFAOYSA-N  
**Formula:** C19H20N2O  
**SMILES:** CC(=O)N1CCN2c3ccccc3Cc3ccccc3C2C1  
**Mol. weight [g/mol]:** 292.37  
**CAS:** 77117-76-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.71		Crippen Method
logp	3.001		Crippen Method
mcvol	230.860	ml/mol	McGowan Method
rmpol	2595.00		NIST Webbook
rmpol	2595.00		NIST Webbook

## Sources

**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=C77117761&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rmpol:** Non-polar retention indices

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