

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

Other names:  
**acetate**

Mianserin M(HO), acetylated

InChI: InChI=1S/C20H22N2O2/c1-14(23)24-17-7-8-19-16(12-17)11-15-5-3-4-6-18(15)20-13-21

InchiKey: UTVHWJCHPKFLAJ-UHFFFAOYSA-N

Formula: C20H22N2O2

SMILES: CC(=O)Oc1ccc2c(c1)Cc1cccc1C1CN(C)CCN21

Mol. weight [g/mol]: 322.40

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.83		Crippen Method
logp	3.009		Crippen Method
mcvol	250.820	ml/mol	McGowan Method
rinpol	2581.00		NIST Webbook
rinpol	2581.00		NIST Webbook

## Sources

McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U280755&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U280755&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemo.com/doc/models/crippen_log10ws">https://www.chemo.com/doc/models/crippen_log10ws</a>

## 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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