2-Methyl-1,2,3,4,9,13b-hexahydro-2,4a-diaza-tribe acetate

Other names:	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)Cc1ccccc1C1CN(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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U280755&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	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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