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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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

Legend

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