2-Acetyl-1,2,3,4,9,13b-hexahydro-2,4a-diaza-triben acetate (ester)

Other names: Mianserin M(Nor-HO), diacetylated
Inchi: InChI=1S/C21H22N2O3/c1-14(24)22-9-10-23-20-8-7-18(26-15(2)25)12-17(20)11-16-5-3-
InchiKey: DVZJGPPXTLDPOK-UHFFFAOYSA-N
Formula: C21H22N2O3
SMILES: CC(=O)Oc1ccc2c(c1)Cc1ccccc1C1CN(C(C)=O)CCN21
Mol. weight [g/mol]: 350.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.03		Crippen Method
logp	2.926		Crippen Method
mcvol	266.480	ml/mol	McGowan Method
rinpol	3005.00		NIST Webbook
rinpol	3005.00		NIST Webbook

Sources

Crippen Method: 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=U280757&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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