

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

Other names: Mian-serin 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
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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

Latest version available from:

<https://www.chemeo.com/cid/96-249-0/2-Acetyl-1-2-3-4-9-13b-hexahydro-2-4a-diaza-tribenzo-a-c-E-cyclohepten-7-ol>

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