2-Acetyl-1,2,3,4,9,13b-hexahydro-2,4a-diaza-triber

Other names: Mianserin M(Nor), acetylated
Inchi: InChI=1S/C19H20N2O/c1-14(22)20-10-11-21-18-9-5-3-7-16(18)12-15-6-2-4-8-17(15)19(
InchiKey: KLGVRKZVHNSAFM-UHFFFAOYSA-N
Formula: C19H20N2O
SMILES: CC(=O)N1CCN2c3ccccc3Cc3ccccc3C2C1
Mol. weight [g/mol]: 292.38

Physical Properties

Property code	Value	Unit	Source
logp	3.001		Crippen Method
mcvol	230.860	ml/mol	McGowan Method
rinpol	2595.00		NIST Webbook
rinpol	2595.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C77117761&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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