Cyclizine M (carbinol), acetylated

Inchi: InChI=1S/C20H24N2O2/c1-17(23)24-20(18-9-5-3-6-10-18,19-11-7-4-8-12-19)22-15-13-2
InchiKey: UPHGJXCMIANUSI-UHFFFAOYSA-N
Formula: C20H24N2O2
SMILES: CC(=O)OC(c1ccccc1)(c1ccccc1)N1CCN(C)CC1
Mol. weight [g/mol]: 324.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Crippen Method
logp	2.698		Crippen Method
mcvol	261.680	ml/mol	McGowan Method
rinpol	1700.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R536302&Units=SI

Legend

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