Azatadine M (nor, OH, -H2O), acetylated

Inchi: InChI=1S/C21H20N2O/c1-15(24)23-13-10-17(11-14-23)20-19-7-3-2-5-16(19)8-9-18-6-4-
InchiKey: BNBLMGRGZSMUEF-UHFFFAOYSA-N
Formula: C21H20N2O
SMILES: CC(=O)N1CCC(=C2c3ccccc3C=Cc3cccnc32)CC1
Mol. weight [g/mol]: 316.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.38		Crippen Method
logp	4.010		Crippen Method
mcvol	250.440	ml/mol	McGowan Method
rinpol	2750.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R120457&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