Azatadine M (nor, OH), acetylated

Inchi: InChI=1S/C23H24N2O3/c1-15(26)25-12-9-17(10-13-25)22-19-7-4-3-6-18(19)14-21(28-16
InchiKey: GQJLCIGGVSTYRD-UHFFFAOYSA-N
Formula: C23H24N2O3
SMILES: CC(=O)OC1Cc2ccccc2C(=C2CCN(C(C)=O)CC2)c2ncccc21
Mol. weight [g/mol]: 376.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.35		Crippen Method
logp	3.686		Crippen Method
mcvol	290.360	ml/mol	McGowan Method
rinpol	2810.00		NIST Webbook
rinpol	2810.00		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=R120442&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.