Azatadine M (OH-aryl), acetylated

Inchi: InChI=1S/C22H24N2O2/c1-15(25)26-19-7-8-20-18(14-19)6-5-17-4-3-11-23-22(17)21(20)
InchiKey: GVSJAOKTXRCZKA-UHFFFAOYSA-N
Formula: C22H24N2O2
SMILES: CC(=O)Oc1ccc2c(c1)CCc1cccnc1C2=C1CCN(C)CC1
Mol. weight [g/mol]: 348.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.31		Crippen Method
logp	3.633		Crippen Method
mcvol	274.700	ml/mol	McGowan Method
rinpol	2540.00		NIST Webbook
rinpol	2540.00		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=R120477&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.