Azatadine M (OH), acetylated

Inchi: InChI=1S/C22H24N2O2/c1-15(25)26-20-14-17-6-3-4-7-18(17)21(16-9-12-24(2)13-10-16)
InchiKey: PCNVUASXUGOEPG-UHFFFAOYSA-N
Formula: C22H24N2O2
SMILES: CC(=O)OC1Cc2ccccc2C(=C2CCN(C)CC2)c2ncccc21
Mol. weight [g/mol]: 348.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.16		Crippen Method
logp	3.769		Crippen Method
mcvol	274.700	ml/mol	McGowan Method
rinpol	2520.00		NIST Webbook
rinpol	2520.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R120462&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

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