

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:	C ₂₁ H ₂₀ N ₂ O
SMILES:	CC(=O)N1CCC(=C2c3ccccc3C=Cc3ccnc32)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
rinsol	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
rinsol:	Non-polar retention indices

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