

Azatadine M (nor), acetylated

Inchi: InChI=1S/C21H22N2O/c1-15(24)23-13-10-17(11-14-23)20-19-7-3-2-5-16(19)8-9-18-6-4-
InchiKey: DUBAGCAHNNYUJQ-UHFFFAOYSA-N
Formula: C21H22N2O
SMILES: CC(=O)N1CCC(=C2c3ccccc3CCc3ccnc32)CC1
Mol. weight [g/mol]: 318.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.19		Crippen Method
logp	3.624		Crippen Method
mcvol	254.740	ml/mol	McGowan Method
rinpola	2720.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R120437&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/40-630-7/Azatadine-M-nor-acetylated.pdf>

Generated by Cheméo on 2024-04-29 03:29:09.386633921 +0000 UTC m=+16650598.307211247.

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