Azatadine M (OH, -H2O)

Inchi: InChI=1S/C20H20N2/c1-22-13-10-16(11-14-22)19-18-7-3-2-5-15(18)8-9-17-6-4-12-21-20
InchiKey: GJUAVAZPKHQKDB-UHFFFAOYSA-N
Formula: C20H20N2
SMILES: CN1CCC(=C2c3ccccc3C=Cc3cccnc32)CC1
Mol. weight [g/mol]: 288.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.19		Crippen Method
logp	4.093		Crippen Method
mcvol	234.780	ml/mol	McGowan Method
rinpol	2410.00		NIST Webbook
rinpol	2410.00		NIST Webbook

Sources

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=R252534&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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