Azatadine

Other names: 5H-Benzo[5,6]cyclohepta[1,2-b]pyridine, 6,11-dihydro-11-(1-methyl-4-piperidinylidene)-
6,11-Dihydro-11-(1-methyl-4-piperidinylidene)-5H-benzo[5,6]cyclohepta[1,2-b]pyridine
Azatidine

Inchi: InChI=1S/C20H22N2/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: SEBMTIQKRHYNIT-UHFFFAOYSA-N

Formula: C20H22N2

SMILES: CN1CCC(=C2c3ccccc3CCc3cccnc32)CC1

Mol. weight [g/mol]: 290.40

CAS: 3964-81-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.00		Crippen Method
logp	3.708		Crippen Method
mcvol	239.080	ml/mol	McGowan Method
rinpol	2375.00		NIST Webbook
rinpol	2368.00		NIST Webbook
rinpol	2415.00		NIST Webbook
rinpol	2375.00		NIST Webbook
rinpol	2368.00		NIST Webbook
rinpol	2415.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3964816&Units=SI

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

Legend

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