

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(=C2c3ccccc3CCc3cccn32)CC1
Mol. weight [g/mol]:	290.41

Physical Properties

Property code	Value	Unit	Source
ie	8.24	eV	Cheméo Relay (1.0)
log10ws	-2.77		Cheméo Relay (1.0)
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	2415.00		NIST Webbook
rinpol	2368.00		NIST Webbook
tf	402.87	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3964816&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rmpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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