Nomelidine

Other names:	(Z)-3-[1-(p-Bromophenyl)-3-(methylamino)propenyl]pyridine
	(Z)-3-(Bromophenyl)-N-methyl-3-(3-pyridyl)-allylamine
	2-Propen-1-amine, 3-(4-bromophenyl)-N-methyl-3-(3-pyridinyl)-, (Z)-
	Norzimelidine
	(Z)-Norzimelidine
	Norzimeldine
Inchi:	InChI=1S/C15H15BrN2/c1-17-10-8-15(13-3-2-9-18-11-13)12-4-6-14(16)7-5-12/h2-9,11,1
InchiKey:	AZFZKANGXPSDEA-NVNXTCNLSA-N
Formula:	C15H15BrN2
SMILES:	CNCC=C(c1ccc(Br)cc1)c1cccnc1
Mol. weight [g/mol]:	303.20
CAS:	60324-59-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.97		Crippen Method
logp	3.495		Crippen Method
mcvol	207.850	ml/mol	McGowan Method
rinpol	2223.00		NIST Webbook
rinpol	2223.00		NIST Webbook
rinpol	2223.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60324596&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