Zimeldine

Other names:	2-Propen-1-amine, 3-(4-bromophenyl)-N,N-dimethyl-3-(3-pyridinyl)-, (Z)- Allylamine, 3-(p-bromophenyl)-N,N-dimethyl-3-(3-pyridyl)-, cis- 3-(4-Bromophenyl)-N,N-dimethyl-3-(3-pyridinyl)-2-propen-1-amine, (Z)- (Z)-3-(4'-Bromophenyl)-3-(3''-pyridyl)dimethylallylamine cis-H 102/09 Zimelidine cis-Zimelidine (Z)-Zimelidine (Z)-3-[1-(p-Bromophenyl)-3-(dimethylamino)propenyl]pyridine H-102/09 (2Z)-3-(4-Bromophenyl)-N,N-dimethyl-3-(3-pyridinyl)-2-propen-1-amine
Inchi:	InChI=1S/C16H17BrN2/c1-19(2)11-9-16(14-4-3-10-18-12-14)13-5-7-15(17)8-6-13/h3-10,
InchiKey:	OYPPVKRFBIWMSX-SXGWCWSVSA-N
Formula:	C16H17BrN2
SMILES:	CN(C)CC=C(c1ccc(Br)cc1)c1cccnc1
Mol. weight [g/mol]:	317.22
CAS:	56775-88-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.77		Crippen Method
logp	3.837		Crippen Method
mcvol	221.940	ml/mol	McGowan Method
rinpol	2206.00		NIST Webbook
rinpol	2206.00		NIST Webbook
rinpol	2206.00		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=C56775883&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