Rotoxamine

Other names:	Ethanamine, 2-[(4-chlorophenyl)-2-pyridinylmethoxy]-N,N-dimethyl-, (-)- l-Carbinoxamine Pyridine, 2-[p-chloro-«alpha»-[2-(dimethylamino)ethoxy]benzyl]-, (-)- ((-))-2-[p-Chloro-«alpha»-[2-(dimethylamino)ethoxy]benzyl]pyridine McN-R-73-Z
Inchi:	InChI=1S/C16H19ClN2O/c1-19(2)11-12-20-16(15-5-3-4-10-18-15)13-6-8-14(17)9-7-13/h
InchiKey:	OJFSXZCBGQGRNV-MRXNPFEDSA-N
Formula:	C16H19ClN2O
SMILES:	CN(C)CCOC(c1ccc(Cl)cc1)c1ccccn1
Mol. weight [g/mol]:	290.79
CAS:	5560-77-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	3.403		Crippen Method
mcvol	226.850	ml/mol	McGowan Method
rinpol	2049.00		NIST Webbook
rinpol	2049.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5560770&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices