Norchloropyramine, acetylated

Inchi: InChI=1S/C17H20ClN3O/c1-14(22)20(2)11-12-21(17-5-3-4-10-19-17)13-15-6-8-16(18)9-

InchiKey: QGDXHDBOTGUHNV-UHFFFAOYSA-N

Formula: C17H20ClN3O

SMILES: CC(=O)N(C)CCN(Cc1ccc(Cl)cc1)c1ccccn1

Mol. weight [g/mol]: 317.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.96		Crippen Method
logp	3.220		Crippen Method
mcvol	246.620	ml/mol	McGowan Method
rinpol	2470.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R536639&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices