

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: QGDHXHDBOTGUHNV-UHFFFAOYSA-N
Formula: C17H20ClN3O
SMILES: CC(=O)N(C)CCN(Cc1ccc(Cl)cc1)c1ccccc1
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/ci990307I>
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

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<https://www.chemeo.com/cid/63-169-5/Norchloropyramine-acetylated.pdf>

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