Chloropyramine, N-desalkyl, acetylated

Inchi: InChI=1S/C14H13ClN2O/c1-11(18)17(14-4-2-3-9-16-14)10-12-5-7-13(15)8-6-12/h2-9H,1
InchiKey: REAVSAMTUGMZRP-UHFFFAOYSA-N
Formula: C14H13ClN2O
SMILES: CC(=O)N(Cc1ccc(Cl)cc1)c1ccccn1
Mol. weight [g/mol]: 260.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.13		Crippen Method
logp	3.288		Crippen Method
mcvol	194.370	ml/mol	McGowan Method
rinpol	2160.00		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=R536159&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