

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)c1cccn1
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
rinpola	2160.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpola:	Non-polar retention indices

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<https://www.chemeo.com/cid/59-936-8/Chloropyramine-N-desalkyl-acetylated.pdf>

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