Chloropyramine, bis-nor, acetylated

Inchi: InChI=1S/C16H18ClN3O/c1-13(21)18-10-11-20(16-4-2-3-9-19-16)12-14-5-7-15(17)8-6-1
InchiKey: RXSKRLSVWTUELL-UHFFFAOYSA-N
Formula: C16H18ClN3O
SMILES: CC(=O)NCCN(Cc1ccc(Cl)cc1)c1ccccn1
Mol. weight [g/mol]: 303.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.16		Crippen Method
logp	2.878		Crippen Method
mcvol	232.530	ml/mol	McGowan Method
rinpol	2420.00		NIST Webbook
rinpol	2420.00		NIST Webbook

Sources

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=R536139&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.