Chloropyramine, hydroxy, acetylated

Inchi: InChI=1S/C18H22ClN3O2/c1-14(23)24-17-8-9-18(20-12-17)22(11-10-21(2)3)13-15-4-6-1
InchiKey: SUOGCEHVUXSRGC-UHFFFAOYSA-N
Formula: C18H22ClN3O2
SMILES: CC(=O)Oc1ccc(N(CCN(C)C)Cc2ccc(Cl)cc2)nc1
Mol. weight [g/mol]: 347.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.08		Crippen Method
logp	3.228		Crippen Method
mcvol	266.580	ml/mol	McGowan Method
rinpol	2440.00		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=R536144&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