Chlorpheniramine M (des-NH2, OH), acetylated

Inchi: InChI=1S/C16H16ClNO2/c1-12(19)20-11-9-15(16-4-2-3-10-18-16)13-5-7-14(17)8-6-13/h
InchiKey: DPOSXBJTCWQDKK-UHFFFAOYSA-N
Formula: C16H16ClNO2
SMILES: CC(=O)OCCC(c1ccc(Cl)cc1)c1ccccn1
Mol. weight [g/mol]: 289.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.52		Crippen Method
logp	3.820		Crippen Method
mcvol	218.440	ml/mol	McGowan Method
rinpol	2130.00		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=R120546&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