

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)c1cccn1
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
rinpola	2130.00		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=R120546&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/19-982-1/Chlorpheniramine-M-des-NH2-OH-acetylated.pdf>

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