Chlorpheniramine M (nor), acetylated

Inchi: InChI=1S/C18H21ClN2O/c1-3-21(14(2)22)13-11-17(18-6-4-5-12-20-18)15-7-9-16(19)10-

InchiKey: PJXVAVRHQXNNLS-UHFFFAOYSA-N

Formula: C18H21ClN2O

SMILES: CCN(CCC(c1ccc(Cl)cc1)c1ccccn1)C(C)=O

Mol. weight [g/mol]: 316.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.84		Crippen Method
logp	4.125		Crippen Method
mcvol	250.730	ml/mol	McGowan Method
rinpol	2530.00		NIST Webbook
rinpol	2530.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R120551&Units=SI

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

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.