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

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