Buclizine M (N-desalkyl), acetylated

Inchi: InChI=1S/C19H21ClN2O/c1-15(23)21-11-13-22(14-12-21)19(16-5-3-2-4-6-16)17-7-9-18(
InchiKey: SQGNETKFPNXNSE-UHFFFAOYSA-N
Formula: C19H21ClN2O
SMILES: CC(=O)N1CCN(C(c2ccccc2)c2ccc(Cl)cc2)CC1
Mol. weight [g/mol]: 328.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.04		Crippen Method
logp	3.594		Crippen Method
mcvol	253.960	ml/mol	McGowan Method
rinpol	2620.00		NIST Webbook
rinpol	2620.00		NIST Webbook
rinpol	2620.00		NIST Webbook
rinpol	2620.00		NIST Webbook
rinpol	2620.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R536124&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