Tripelenamine M (nor-hydroxy), acetylated

Inchi: InChI=1S/C19H23N3O3/c1-15(23)21(3)12-13-22(19-6-4-5-11-20-19)14-17-7-9-18(10-8-1
InchiKey: UFIYMAFCSLYORZ-UHFFFAOYSA-N
Formula: C19H23N3O3
SMILES: CC(=O)Oc1ccc(CN(CCN(C)C(C)=O)c2ccccn2)cc1
Mol. weight [g/mol]: 341.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	2.492		Crippen Method
mcvol	270.000	ml/mol	McGowan Method
rinpol	2860.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R536728&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices