Tripelenamine M (hydroxy), acetylated

Inchi: InChI=1S/C18H23N3O2/c1-15(22)23-17-9-7-16(8-10-17)14-21(13-12-20(2)3)18-6-4-5-11
InchiKey: NJISWQNABFGSMO-UHFFFAOYSA-N
Formula: C18H23N3O2
SMILES: CC(=O)Oc1ccc(CN(CCN(C)C)c2ccccn2)cc1
Mol. weight [g/mol]: 313.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.39		Crippen Method
logp	2.575		Crippen Method
mcvol	254.340	ml/mol	McGowan Method
rinpol	2390.00		NIST Webbook
rinpol	2390.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R536708&Units=SI

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.