Tripelenamine M (nor), acetylated

Inchi: InChI=1S/C17H21N3O/c1-15(21)19(2)12-13-20(17-10-6-7-11-18-17)14-16-8-4-3-5-9-16/h
InchiKey: FVUSGFONCNEWBN-UHFFFAOYSA-N
Formula: C17H21N3O
SMILES: CC(=O)N(C)CCN(Cc1ccccc1)c1ccccn1
Mol. weight [g/mol]: 283.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.27		Crippen Method
logp	2.567		Crippen Method
mcvol	234.380	ml/mol	McGowan Method
rinpol	2420.00		NIST Webbook
rinpol	2420.00		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=R536713&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.