Mepyramine M (N-desalkyl), acetylated

Inchi: InChI=1S/C15H16N2O2/c1-12(18)17(15-5-3-4-10-16-15)11-13-6-8-14(19-2)9-7-13/h3-10
InchiKey: DZTCRDKYMKRASV-UHFFFAOYSA-N
Formula: C15H16N2O2
SMILES: COc1ccc(CN(C(C)=O)c2ccccn2)cc1
Mol. weight [g/mol]: 256.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	2.643		Crippen Method
mcvol	202.090	ml/mol	McGowan Method
rinpol	2150.00		NIST Webbook
rinpol	2150.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R536580&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.