Trimipramime M(HO), acetylated

Inchi: InChI=1S/C22H28N2O2/c1-16(14-23(3)4)15-24-21-8-6-5-7-18(21)9-10-19-11-12-20(13-2
InchiKey: HULUZCZCSNSROU-UHFFFAOYSA-N
Formula: C22H28N2O2
SMILES: CC(=O)Oc1ccc2c(c1)N(CC(C)CN(C)C)c1ccccc1CC2
Mol. weight [g/mol]: 352.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.57		Crippen Method
logp	4.046		Crippen Method
mcvol	289.860	ml/mol	McGowan Method
rinpol	2652.00		NIST Webbook

Sources

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=R311232&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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