

Trimipramine M(Nor-HO), diacetylated

Inchi: InChI=1S/C23H28N2O3/c1-16(14-24(4)17(2)26)15-25-22-8-6-5-7-19(22)9-10-20-11-12-2
InchiKey: IMHSJSNUBJQJQK-UHFFFAOYSA-N
Formula: C23H28N2O3
SMILES: CC(=O)Oc1ccc2c(c1)N(CC(C)CN(C)C(C)=O)c1cccc1CC2
Mol. weight [g/mol]: 380.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.77		Crippen Method
logp	3.963		Crippen Method
mcvol	305.520	ml/mol	McGowan Method
rinpol	3153.00		NIST Webbook
rinpol	3153.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R311252&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

Latest version available from:

<https://www.chemeo.com/cid/14-146-4/Trimipramine-M-Nor-HO-diacetylated.pdf>

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