

Trimipramine M(Nor-di-HO), triacetylated

Inchi:	InChI=1S/C25H30N2O5/c1-16(14-26(5)17(2)28)15-27-24-11-10-22(31-18(3)29)12-21(24
InchiKey:	SFPDXOGPRMPSAW-UHFFFAOYSA-N
Formula:	C25H30N2O5
SMILES:	CC(=O)Oc1ccc2c(c1)CCc1ccc(OC(C)=O)cc1N2CC(C)CN(C)C(C)=O
Mol. weight [g/mol]:	438.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.08		Crippen Method
logp	3.888		Crippen Method
mcvol	341.140	ml/mol	McGowan Method
rinsol	3556.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R311247&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinsol:	Non-polar retention indices

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<https://www.chemeo.com/cid/11-867-7/Trimipramine-M-Nor-di-HO-triacetylated.pdf>

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