Desipramine M(HO), acetylated

Inchi: InChI=1S/C22H26N2O3/c1-16(25)23(3)13-6-14-24-21-8-5-4-7-18(21)9-10-19-15-20(27-1
InchiKey: JJZGYDOWGFFLQG-UHFFFAOYSA-N
Formula: C22H26N2O3
SMILES: CC(=O)Oc1ccc2c(c1)CCc1ccccc1N2CCCN(C)C(C)=O
Mol. weight [g/mol]: 366.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.59		Crippen Method
logp	3.717		Crippen Method
mcvol	291.430	ml/mol	McGowan Method
rinpol	3066.00		NIST Webbook
rinpol	3066.00		NIST Webbook
rinpol	3066.00		NIST Webbook
rinpol	3066.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310848&Units=SI
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

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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