Clomipramine M(Nor-HO), diacetylated

Inchi: InChI=1S/C22H25ClN2O3/c1-15(26)24(3)11-4-12-25-21-10-9-20(28-16(2)27)13-18(21)6-

InchiKey: PWHSPXYSWCJWEW-UHFFFAOYSA-N

Formula: C22H25ClN2O3

SMILES: CC(=O)Oc1ccc2c(c1)CCc1ccc(Cl)cc1N2CCCN(C)C(C)=O

Mol. weight [g/mol]: 400.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.28		Crippen Method
logp	4.370		Crippen Method
mcvol	303.670	ml/mol	McGowan Method
rinpol	3205.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310813&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