

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

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<https://www.chemeo.com/cid/20-972-0/Clomipramine-M-Nor-HO-diacetylated.pdf>

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