

Clomipramine M(HO), acetylated, isomer # 2

Inchi: InChI=1S/C21H25ClN2O2/c1-15(25)26-19-9-10-20-17(13-19)6-5-16-7-8-18(22)14-21(16)
InchiKey: SMWFCHXREKPVEY-UHFFFAOYSA-N
Formula: C21H25ClN2O2
SMILES: CC(=O)Oc1ccc2c(c1)CCc1ccc(Cl)cc1N2CCCN(C)C
Mol. weight [g/mol]: 372.89

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.08		Crippen Method
logp	4.454		Crippen Method
mcvol	288.010	ml/mol	McGowan Method
rinsol	2906.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R310799&Units=SI>

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.cheméo.com/cid/119-896-6/Clomipramine-M-HO-acetylated-isomer-2.pdf>

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