

# Clomipramine N(HO), acetylated, isomer # 1

**Inchi:** InChI=1S/C21H25ClN2O2/c1-15(25)26-20-7-4-6-17-9-8-16-10-11-18(22)14-19(16)24(21)23  
**InchiKey:** DJAMHNZZGJVDEU-UHFFFAOYSA-N  
**Formula:** C<sub>21</sub>H<sub>25</sub>ClN<sub>2</sub>O<sub>2</sub>  
**SMILES:** CC(=O)Oc1cccc2c1N(CCCN(C)C)c1cc(Cl)ccc1CC2  
**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	2806.00		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](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=R310828&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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