

# Mirtazapine-M (nor-HO-methoxy-) 2AC

**Inchi:** InChI=1S/C21H23N3O4/c1-13(25)23-6-7-24-20(12-23)19-5-4-17(28-14(2)26)9-15(19)8-1  
**InchiKey:** RNUGXCVWLPMCCT-UHFFFAOYSA-N  
**Formula:** C21H23N3O4  
**SMILES:** COc1cnc2c(c1)Cc1cc(OC(C)=O)ccc1C1CN(C(C)=O)CCN21  
**Mol. weight [g/mol]:** 381.43

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.91		Crippen Method
logp	2.329		Crippen Method
mcvol	282.330	ml/mol	McGowan Method
rinpola	3195.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.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=R331083&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpola:** Non-polar retention indices

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