

# Paroxetine, N-acetyl-

**Other names:** Paroxetine, acetyl  
**Inchi:** InChI=1S/C21H22FNO4/c1-14(24)23-9-8-19(15-2-4-17(22)5-3-15)16(11-23)12-25-18-6-7  
**InchiKey:** UQXZOFZRYGCMY-UHFFFAOYSA-N  
**Formula:** C21H22FNO4  
**SMILES:** CC(=O)N1CCC(c2ccc(F)cc2)C(COc2ccc3c(c2)OCO3)C1  
**Mol. weight [g/mol]:** 371.40

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.64		Crippen Method
logp	3.585		Crippen Method
mcvol	268.440	ml/mol	McGowan Method
rmpol	2980.00		NIST Webbook
rmpol	2980.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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=U308751&Units=SI>

## Legend

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

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