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: UQXZOFZRYGCMMY-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
rinpol	2980.00		NIST Webbook
rinpol	2980.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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
rinpol: Non-polar retention indices