Paroxetine, demethylenyl-3-methyl, diacetyl

Inchi: InChI=1S/C23H26FNO5/c1-15(26)25-11-10-21(17-4-6-19(24)7-5-17)18(13-25)14-29-20-8
InchiKey: HVHLZOHPNYXMKO-WIYYLYMNSA-N
Formula: C23H26FNO5
SMILES: COc1cc(OCC2CN(C(C)=O)CCC2c2ccc(F)cc2)ccc1OC(C)=O
Mol. weight [g/mol]: 415.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.86		Crippen Method
logp	3.791		Crippen Method
mcvol	309.050	ml/mol	McGowan Method
rinpol	3030.00		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=R196033&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