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

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