Moexipril desethyl - H2O Me (Moexprilate - H2O Me)

Inchi: InChI=1S/C27H32N2O6/c1-5-35-27(32)21(12-11-18-9-7-6-8-10-18)29-17(2)25(30)28-16-

InchiKey: UYPPDNXTLSUNRF-ZPMCFJSWSA-N

Formula: C27H32N2O6

SMILES: CCOC(=O)C(CCc1ccccc1)N1C(=O)C2Cc3cc(OC)c(OC)cc3CN2C(=O)C1C

Mol. weight [g/mol]: 480.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.87		Crippen Method
logp	2.752		Crippen Method
mcvol	364.330	ml/mol	McGowan Method
rinpol	3775.00		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=R549907&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