Moexipril desethyl 3Me (Moexprilate 3Me)

Inchi: InChI=1S/C28H36N2O7/c1-18(29(2)22(27(32)36-5)13-12-19-10-8-7-9-11-19)26(31)30-17
InchiKey: OHLVOLSWNRERQE-SXSPYAJSSA-N
Formula: C28H36N2O7
SMILES: COC(=O)C1Cc2cc(OC)c(OC)cc2CN1C(=O)C(C)N(C)C(CCc1ccccc1)C(=O)OC
Mol. weight [g/mol]: 512.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.48		Crippen Method
logp	2.625		Crippen Method
mcvol	395.150	ml/mol	McGowan Method
rinpol	3580.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R549898&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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