Moexipril Me

Inchi: InChI=1S/C29H38N2O7/c1-7-38-29(34)23(14-13-20-11-9-8-10-12-20)30(3)19(2)27(32)31
InchiKey: RATQLCAPWCNXSQ-CTUHWIOQSA-N
Formula: C29H38N2O7
SMILES: CCOC(=O)C(CCc1ccccc1)N(C)C(C)C(=O)N1Cc2cc(OC)c(OC)cc2CC1C(=O)OC
Mol. weight [g/mol]: 526.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.90		Crippen Method
logp	3.015		Crippen Method
mcvol	409.240	ml/mol	McGowan Method
rinpol	3575.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R549912&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