Quinapril Me

Inchi: InChI=1S/C27H34N2O5/c1-5-34-27(32)23(16-15-20-11-7-6-8-12-20)28(3)19(2)25(30)29-
InchiKey: NBNFTJZLRIMKOI-NXJLTJBGSA-N
Formula: C27H34N2O5
SMILES: CCOC(=O)C(CCc1ccccc1)N(C)C(C)C(=O)N1Cc2ccccc2CC1C(=O)OC
Mol. weight [g/mol]: 466.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.66		Crippen Method
logp	2.998		Crippen Method
mcvol	369.320	ml/mol	McGowan Method
rinpol	3110.00		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=R549972&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