Quinapril desethyl 3Me (Quinaprilate 3Me)

Inchi: InChI=1S/C26H32N2O5/c1-18(27(2)22(25(30)32-3)15-14-19-10-6-5-7-11-19)24(29)28-17
InchiKey: JQDMJLSGNWHRJP-OFSKKJKASA-N
Formula: C26H32N2O5
SMILES: COC(=O)C1Cc2ccccc2CN1C(=O)C(C)N(C)C(CCc1ccccc1)C(=O)OC
Mol. weight [g/mol]: 452.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.24		Crippen Method
logp	2.608		Crippen Method
mcvol	355.230	ml/mol	McGowan Method
rinpol	3080.00		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=R549952&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