Benazepril desethyl 3Me (Benazeprilate 3Me)

Inchi: InChI=1S/C25H30N2O5/c1-26(22(25(30)32-3)15-13-18-9-5-4-6-10-18)21-16-14-19-11-7-

InchiKey: OITBKUHYWGZZHQ-FGZHOGPDSA-N

Formula: C25H30N2O5

SMILES: COC(=O)CN1C(=O)C(N(C)C(CCc2ccccc2)C(=O)OC)CCc2ccccc21

Mol. weight [g/mol]: 438.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.75		Crippen Method
logp	2.614		Crippen Method
mcvol	341.140	ml/mol	McGowan Method
rinpol	2985.00		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=R549818&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