Benazepril Me

Inchi: InChI=1S/C25H30N2O5/c1-3-32-25(30)21(15-13-18-9-5-4-6-10-18)26-20-16-14-19-11-7-
InchiKey: NQJYCOHSACSXSO-NHCUHLMSSA-N
Formula: C25H30N2O5
SMILES: CCOC(=O)C(CCc1ccccc1)NC1CCc2ccccc2N(CC(=O)OC)C1=O
Mol. weight [g/mol]: 438.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.37		Crippen Method
logp	2.662		Crippen Method
mcvol	341.140	ml/mol	McGowan Method
rinpol	3030.00		NIST Webbook
rinpol	3030.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R549823&Units=SI
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

Legend

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

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