

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R549818&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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