

Enalapril desethyl - H2O, Me (Enalaprilate - H2O, Me)

Inchi: InChI=1S/C19H24N2O4/c1-13-17(22)20-12-6-9-15(20)18(23)21(13)16(19(24)25-2)11-10
InchiKey: CQOAAQPDP RERPP-FVQBIDKESA-N
Formula: C19H24N2O4
SMILES: COC(=O)C(CCCc1cccc1)N1C(=O)C2CCCN2C(=O)C1C
Mol. weight [g/mol]: 344.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	1.383		Crippen Method
mcvol	263.630	ml/mol	McGowan Method
rinsol	2735.00		NIST Webbook

Sources

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=R549863&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/33-395-7/Enalapril-desethyl-H2O-Me-Enalaprilate-H2O-Me.pdf>

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