

Enalapril Me

Inchi: InChI=1S/C21H30N2O5/c1-4-28-20(25)17(13-12-16-9-6-5-7-10-16)22-15(2)19(24)23-14
InchiKey: WCGKQGYHVTZCIZ-KBAYOESNSA-N
Formula: C21H30N2O5
SMILES: CCOC(=O)C(CCc1ccccc1)NC(C)C(=O)N1CCCC1C(=O)OC
Mol. weight [g/mol]: 390.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.21		Crippen Method
logp	1.693		Crippen Method
mcvol	308.540	ml/mol	McGowan Method
rinsol	2675.00		NIST Webbook
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Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R549878&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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