

Enalapril desethyl 3Me (Enalaprilate 3Me)

Inchi:	InChI=1S/C21H30N2O5/c1-15(19(24)23-14-8-11-18(23)21(26)28-4)22(2)17(20(25)27-3)
InchiKey:	XSAARGUZTCURKI-KBAYOESNSA-N
Formula:	C21H30N2O5
SMILES:	<chem>COC(=O)C1CCCN1C(=O)C(C)N(C)C(Cc1ccccc1)C(=O)OC</chem>
Mol. weight [g/mol]:	390.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.59		Crippen Method
logp	1.645		Crippen Method
mcvol	308.540	ml/mol	McGowan Method
rmpol	2680.00		NIST Webbook
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R549858&Units=SI

Legend

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

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