

Moexipril desethyl - H2O Me (Moexprilate - H2O Me)

Inchi: InChI=1S/C27H32N2O6/c1-5-35-27(32)21(12-11-18-9-7-6-8-10-18)29-17(2)25(30)28-16-3
InchiKey: UYPPDNXTLSUNRF-ZPMCFSWSA-N
Formula: C27H32N2O6
SMILES: CCOC(=O)C(CCCc1ccccc1)N1C(=O)C2Cc3cc(OC)c(OC)cc3CN2C(=O)C1C
Mol. weight [g/mol]: 480.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.87		Crippen Method
logp	2.752		Crippen Method
mcvol	364.330	ml/mol	McGowan Method
rinpol	3775.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R549907&Units=SI>

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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