

Cilazapril Me

Inchi: InChI=1S/C24H35N3O5/c1-4-32-24(30)20(15-14-18-10-6-5-7-11-18)25(2)19-12-8-16-26
InchiKey: RTTXUCGGFZMPJT-AHTKWCMKSA-N
Formula: C24H35N3O5
SMILES: CCOC(=O)C(CCc1ccccc1)N(C)C1CCCN2CCCC(C(=O)OC)N2C1=O
Mol. weight [g/mol]: 445.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.30		Crippen Method
logp	2.026		Crippen Method
mcvol	349.930	ml/mol	McGowan Method
rinpol	3010.00		NIST Webbook
rinpol	3010.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R549843&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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<https://www.chemeo.com/cid/18-874-2/Cilazapril-Me.pdf>

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