

Cilazapril desethyl 3Me (Cilazaprilate 3Me)

Inchi: InChI=1S/C23H33N3O5/c1-24(19(22(28)30-2)14-13-17-9-5-4-6-10-17)18-11-7-15-25-16
InchiKey: VDYOLOGIYNYEBQ-NFBCFJMWSA-N
Formula: C23H33N3O5
SMILES: COC(=O)C(CCC1CCCCC1)N(C)C1CCCN2CCCC(C(=O)OC)N2C1=O
Mol. weight [g/mol]: 431.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.88		Crippen Method
logp	1.636		Crippen Method
mcvol	335.840	ml/mol	McGowan Method
rinpol	2960.00		NIST Webbook
rinpol	2960.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R549838&Units=SI>
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>

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/16-275-9/Cilazapril-desethyl-3Me-Cilazaprilate-3Me.pdf>

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