Seneciphylline, 12-acetyl

Inchi: InChI=1S/C20H25NO6/c1-5-14-10-12(2)20(4,27-13(3)22)19(24)25-11-15-6-8-21-9-7-16(1
InchiKey: CTCKXBIRQMSUIU-BYVYPXNKSA-N
Formula: C20H25NO6
SMILES: C=C1CC(=CC)C(=O)OC2CCN3CC=C(COC(=O)C1(C)OC(C)=O)C23
Mol. weight [g/mol]: 375.42

Physical Properties

Property code	Value	Unit	Source
logp	1.684		Crippen Method
mcvol	279.480	ml/mol	McGowan Method
rinpol	2531.00		NIST Webbook
rinpol	2531.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R636670&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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