

Seneciophylline, 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(3)
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
log10ws	-2.93		Crippen Method
logp	1.684		Crippen Method
mcvol	279.480	ml/mol	McGowan Method
rinpol	2531.00		NIST Webbook
rinpol	2531.00		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=R636670&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

Latest version available from:

<https://www.chemeo.com/cid/97-870-9/Seneciophylline-12-acetyl.pdf>

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