7-senecioyllycopsamine

Inchi: InChI=1S/C20H31NO6/c1-12(2)10-17(23)27-14(5)20(25,13(3)4)19(24)26-11-15-6-8-21-9
InchiKey: PMVFQLSWVIQZGK-CQEAQJRCSA-N
Formula: C20H31NO6
SMILES: CC(C)=CC(=O)OC(C)C(O)(C(=O)OCC1=CCN2CCC(O)C12)C(C)C
Mol. weight [g/mol]: 381.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.72		Crippen Method
logp	1.190		Crippen Method
mcvol	298.940	ml/mol	McGowan Method
rinpol	2497.00		NIST Webbook
rinpol	2495.00		NIST Webbook
rinpol	2495.00		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=R299602&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