Senecionine, 12-acetyl

Inchi:	InChI=1S/C20H27NO6/c1-5-14-10-12(2)20(4,27-13(3)22)19(24)25-11-15-6-8-21-9-7-16(
InchiKey:	IVYWMLHULLVCRQ-ORELLFKUSA-N
Formula:	C20H27NO6
SMILES:	CC=C1CC(C)C(C)(OC(C)=O)C(=O)OCC2=CCN3CCC(OC1=O)C23
Mol. weight [g/mol]:	377.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.84		Crippen Method
logp	1.764		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
rinpol	2505.00		NIST Webbook
rinpol	2505.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R636665&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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