

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(3)
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
rinpola	2505.00		NIST Webbook
rinpola	2505.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R636665&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

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