3'-acetylechiupinine

Inchi: InChI=1S/C22H33NO7/c1-13(2)11-19(25)30-18-8-10-23-9-7-17(20(18)23)12-28-21(26)22
InchiKey: DJSXKISBHKHRKA-LAKFJOCUSA-N
Formula: C22H33NO7
SMILES: CC(=O)OC(C)C(O)(C(=O)OCC1=CCN2CCC(OC(=O)C=C(C)C)C12)C(C)C
Mol. weight [g/mol]: 423.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.16		Crippen Method
logp	1.761		Crippen Method
mcvol	328.690	ml/mol	McGowan Method
rinpol	2557.00		NIST Webbook
rinpol	2557.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R516457&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.