3'-dihydrocinnamoylindicine

Inchi: InChI=1S/C24H33NO6/c1-16(2)24(29,17(3)31-21(27)10-9-18-7-5-4-6-8-18)23(28)30-15-1
InchiKey: FYDBMEDXSGLGIR-MFHCRVQTSA-N
Formula: C24H33NO6
SMILES: CC(C)C(O)(C(=O)OCC1=CCN2CCC(O)C12)C(C)OC(=O)CCc1ccccc1
Mol. weight [g/mol]: 431.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.64		Crippen Method
logp	1.856		Crippen Method
mcvol	335.840	ml/mol	McGowan Method
rinpol	2910.00		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=R516506&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