9-Angeloylanacrotine

Inchi: InChI=1S/C23H31NO6/c1-6-14(3)20(25)30-23(5)15(4)12-16(7-2)21(26)29-18-9-11-24-10
InchiKey: MGQIZYQQEVSTTF-YZMKKPCBSA-N
Formula: C23H31NO6
SMILES: CC=C(C)C(=O)OC1(C)C(=O)OCC2=CCN3CCC(OC(=O)C(=CC)CC1C)C23
Mol. weight [g/mol]: 417.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.95		Crippen Method
logp	2.710		Crippen Method
mcvol	321.750	ml/mol	McGowan Method
rinpol	2858.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R405253&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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