7-Angeloyl-9-(2-methylbutyryl)heliotridine

Inchi: InChI=1S/C18H27NO4/c1-5-12(3)17(20)22-11-14-7-9-19-10-8-15(16(14)19)23-18(21)13(
InchiKey: HCWYTYBGRVJHCP-HCEHKAJUSA-N
Formula: C18H27NO4
SMILES: CC=C(C)C(=O)OC1CCN2CC=C(COC(=O)C(C)CC)C12
Mol. weight [g/mol]: 321.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.13		Crippen Method
logp	2.468		Crippen Method
mcvol	259.020	ml/mol	McGowan Method
rinpol	2183.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R299657&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