7-Angeloyl-9-(2,3-dihydroxylbutyryl)heliotridine

Inchi: InChI=1S/C17H25NO6/c1-4-10(2)16(21)24-13-6-8-18-7-5-12(14(13)18)9-23-17(22)15(20
InchiKey: RXOCMPDBRBLXGB-MZWYSVSMSA-N
Formula: C17H25NO6
SMILES: CC=C(C)C(=O)OC1CCN2CC=C(COC(=O)C(O)C(C)O)C12
Mol. weight [g/mol]: 339.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.71		Crippen Method
logp	0.164		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
rinpol	2333.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R299642&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