7-Angeloyl-9-(hydroxypropenoyl) retronecine

Inchi: InChI=1S/C16H23NO5/c1-4-10(2)15(19)22-13-6-8-17-7-5-12(14(13)17)9-21-16(20)11(3)
InchiKey: LFJWMCVWUAPRBO-BXOSMATJSA-N
Formula: C16H23NO5
SMILES: C=C(O)C(=O)OCC1CCN2CCC(OC(=O)C(C)=CC)C12
Mol. weight [g/mol]: 309.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.11		Crippen Method
logp	1.574		Crippen Method
mcvol	236.710	ml/mol	McGowan Method
rinpol	2053.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R227860&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