7-angeloyl-9-(2,3-dihydroxy propanoyl) retronecine

Inchi: InChI=1S/C16H25NO6/c1-3-10(2)15(20)23-13-5-7-17-6-4-11(14(13)17)9-22-16(21)12(19

InchiKey: UCZOPSUTRUWZNY-NQQHZPIASA-N

Formula: C16H25NO6

SMILES: CC=C(C)C(=O)OC1CCN2CCC(COC(=O)C(O)CO)C12

Mol. weight [g/mol]: 327.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.08		Crippen Method
logp	-0.145		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
rinpol	2300.00		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=R227855&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

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