9-Angeloylretronecine

Inchi: InChI=1S/C13H19NO3/c1-3-9(2)13(16)17-8-10-4-6-14-7-5-11(15)12(10)14/h3-4,11-12,15
InchiKey: VYUQPLFRNDQDHW-KKXNAPIPSA-N
Formula: C13H19NO3
SMILES: CC=C(C)C(=O)OCC1=CCN2CCC(O)C12
Mol. weight [g/mol]: 237.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.68		Crippen Method
logp	0.871		Crippen Method
mcvol	187.000	ml/mol	McGowan Method
rinpol	1840.00		NIST Webbook
rinpol	1795.00		NIST Webbook
rinpol	1797.00		NIST Webbook
rinpol	1797.00		NIST Webbook
rinpol	1797.00		NIST Webbook
rinpol	1797.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R178040&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