7-tigloylretronecine

Inchi: InChI=1S/C13H19NO3/c1-3-9(2)13(16)17-11-5-7-14-6-4-10(8-15)12(11)14/h3-4,11-12,15
InchiKey: TYGYPIIOOQNWBU-ZSBMJCTGSA-N
Formula: C13H19NO3
SMILES: CC=C(C)C(=O)OC1CCN2CC=C(CO)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	1815.00		NIST Webbook
rinpol	1858.00		NIST Webbook
rinpol	1815.00		NIST Webbook
rinpol	1815.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R178035&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

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