9-tigloylretronecine

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-UHTQEIBISA-N
Formula: C13H19NO3
SMILES: C/C=C(\C)C(=O)OCC1=CCN2CC[C@@H](O)[C@@H]12
Mol. weight [g/mol]: 237.30

Physical Properties

Property code	Value	Unit	Source
logp	0.871		Crippen Method
mcvol	187.000	ml/mol	McGowan Method
rinpol	1845.00		NIST Webbook
rinpol	1842.00		NIST Webbook
rinpol	1852.00		NIST Webbook
rinpol	1888.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R177854&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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https://www.chemeo.com/cid/48-841-5/9-tigloylretronecine.pdf

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