7-acetyl-9-sarracinoylretronecine

Inchi: InChI=1S/C15H21NO4/c1-10(2)8-14(18)19-9-12-4-6-16-7-5-13(15(12)16)20-11(3)17/h4,8

InchiKey: WGEMRYCTYCCJMA-ZFWWWQNUSA-N

Formula: C15H21NO4

SMILES: CC(=O)OC1CCN2CC=C(COC(=O)C=C(C)C)C12

Mol. weight [g/mol]: 279.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.12		Crippen Method
logp	1.442		Crippen Method
mcvol	216.750	ml/mol	McGowan Method
rinpol	2125.00		NIST Webbook
rinpol	2125.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R227835&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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