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

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=R227835&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.