7-acetyl-9-(2-hydroxy-3-methylbutyryl) retronecine

Inchi: InChI=1S/C15H23NO5/c1-9(2)14(18)15(19)20-8-11-4-6-16-7-5-12(13(11)16)21-10(3)17/h

InchiKey: OTEHYFUSZSWPPU-HSBZDZAISA-N

Formula: C15H23NO5

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

Mol. weight [g/mol]: 297.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.40		Crippen Method
logp	0.493		Crippen Method
mcvol	226.920	ml/mol	McGowan Method
rinpol	2024.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R240521&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices