7-acetyl-9-(2,3-dihydroxybutyryl) retronecine

Inchi: InChI=1S/C14H21NO6/c1-8(16)13(18)14(19)20-7-10-3-5-15-6-4-11(12(10)15)21-9(2)17/h
InchiKey: NSVBJEHUKQDBMA-UASQIEKGSA-N
Formula: C14H21NO6
SMILES: CC(=O)OC1CCN2CC=C(COC(=O)C(O)C(C)O)C12
Mol. weight [g/mol]: 299.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.60		Crippen Method
logp	-0.783		Crippen Method
mcvol	218.700	ml/mol	McGowan Method
rinpol	2092.00		NIST Webbook
rinpol	2092.00		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=R240501&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.