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

Inchi: InChI=1S/C15H23NO4/c1-4-10(2)15(18)19-9-12-5-7-16-8-6-13(14(12)16)20-11(3)17/h5,1
InchiKey: TXLFMEAPKXAGPH-AWAWDMARSA-N
Formula: C15H23NO4
SMILES: CCC(C)C(=O)OCC1=CCN2CCC(OC(C)=O)C12
Mol. weight [g/mol]: 281.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.02		Crippen Method
logp	1.522		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
rinpol	1914.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R240536&Units=SI
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

Legend

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