7-(2-Methylbutyryl)-retronecine

Inchi: InChI=1S/C13H21NO3/c1-3-9(2)13(16)17-11-5-7-14-6-4-10(8-15)12(11)14/h4,9,11-12,15
InchiKey: NSBSOFPYQQNEGC-ZYXZCXLHSA-N
Formula: C13H21NO3
SMILES: CCC(C)C(=O)OC1CCN2CC=C(CO)C12
Mol. weight [g/mol]: 239.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.59		Crippen Method
logp	0.951		Crippen Method
mcvol	191.300	ml/mol	McGowan Method
rinpol	1738.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R299588&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