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

Inchi: InChI=1S/C13H21NO4/c1-8(2)12(16)13(17)18-7-9-3-4-14-6-10(15)5-11(9)14/h3,8,10-12,
InchiKey: VZLCAAPCARGWDL-UHFFFAOYSA-N
Formula: C13H21NO4
SMILES: CC(C)C(O)C(=O)OCC1=CCN2CC(O)CC12
Mol. weight [g/mol]: 255.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.96		Crippen Method
logp	-0.078		Crippen Method
mcvol	197.170	ml/mol	McGowan Method
rinpol	1835.00		NIST Webbook
rinpol	1835.00		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=R178342&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

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