7-acetylretronecine

Inchi: InChI=1S/C10H15NO3/c1-7(13)14-9-3-5-11-4-2-8(6-12)10(9)11/h2,9-10,12H,3-6H2,1H3/
InchiKey: HMVVLENFARUUJW-RGURZIINSA-N
Formula: C10H15NO3
SMILES: CC(=O)OC1CCN2CC=C(CO)C12
Mol. weight [g/mol]: 197.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.57		Crippen Method
logp	-0.075		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
rinpol	1532.00		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=R240541&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