9-Methyl-didehydroretronecine

Inchi: InChI=1S/C9H13NO2/c1-6(11)7-2-4-10-5-3-8(12)9(7)10/h2-3,5-6,8-9,11-12H,4H2,1H3/t6
InchiKey: YJKQQMLYODPAMA-XNGKIHLYSA-N
Formula: C9H13NO2
SMILES: CC(O)C1=CCN2C=CC(O)C12
Mol. weight [g/mol]: 167.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.01		Crippen Method
logp	-0.134		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
rinpol	1387.00		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=R283162&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