3«alpha»-Isobutyroxytropane

Inchi: InChI=1S/C12H21NO2/c1-8(2)12(14)15-11-6-9-4-5-10(7-11)13(9)3/h8-11H,4-7H2,1-3H3/
InchiKey: UAINLAXRDPKCOO-URLYPYJESA-N
Formula: C12H21NO2
SMILES: CC(C)C(=O)OC1CC2CCC(C1)N2C
Mol. weight [g/mol]: 211.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.16		Crippen Method
logp	1.811		Crippen Method
mcvol	175.640	ml/mol	McGowan Method
rinpol	1455.00		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=R509518&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