3«beta»-(Hydroxypentanoyloxy)tropane

Inchi: InChI=1S/C13H23NO3/c1-3-4-12(15)13(16)17-11-7-9-5-6-10(8-11)14(9)2/h9-12,15H,3-8
InchiKey: JAOVXKLIJXRSEI-VBLDAPLVSA-N
Formula: C13H23NO3
SMILES: CCCC(O)C(=O)OC1CC2CCC(C1)N2C
Mol. weight [g/mol]: 241.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.20		Crippen Method
logp	1.316		Crippen Method
mcvol	195.600	ml/mol	McGowan Method
rinpol	1552.00		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=R509667&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