3-Propionyloxy-6-hydroxytropane

Inchi: InChI=1S/C11H19NO3/c1-3-11(14)15-8-4-7-5-10(13)9(6-8)12(7)2/h7-10,13H,3-6H2,1-2H
InchiKey: GWIDTVSZSPYVQH-QGVKSAJWSA-N
Formula: C11H19NO3
SMILES: CCC(=O)OC1CC2CC(O)C(C1)N2C
Mol. weight [g/mol]: 213.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.36		Crippen Method
logp	0.536		Crippen Method
mcvol	167.420	ml/mol	McGowan Method
rinpol	1538.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R421651&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices