

3«alpha»-Hydroxy-6«beta»-acetoxytropane

Inchi:	InChI=1S/C9H15NO3/c1-6(11)13-5-10-7-2-8(10)4-9(12)3-7/h7-9,12H,2-5H2,1H3/t7-,8?,9
InchiKey:	PCTJRBGXKRLHY-NBXIYJJMSA-N
Formula:	C9H15NO3
SMILES:	CC(=O)OCN1C2CC(O)CC1C2
Mol. weight [g/mol]:	185.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.91		Crippen Method
logp	0.105		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
rinpol	1409.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R421408&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

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