3«alpha»-Acetoxytropane

Inchi: InChI=1S/C10H17NO2/c1-7(12)13-10-5-8-3-4-9(6-10)11(8)2/h8-10H,3-6H2,1-2H3/t8-,9+,
InchiKey: MDIDMOWWLBGYPG-MYJAWHEDSA-N
Formula: C10H17NO2
SMILES: CC(=O)OC1CC2CCC(C1)N2C
Mol. weight [g/mol]: 183.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.57		Crippen Method
logp	1.175		Crippen Method
mcvol	147.460	ml/mol	McGowan Method
rinpol	1340.00		NIST Webbook
rinpol	1341.00		NIST Webbook
rinpol	1303.00		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1308.00		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=R411144&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