

3-(Hydroxyacetoxy)-tropane

Inchi: InChI=1S/C10H17NO3/c1-11-7-2-3-8(11)5-9(4-7)14-10(13)6-12/h7-9,12H,2-6H2,1H3/t7-
InchiKey: IAWYYJRDAMGQCB-JVHMLUBASA-N
Formula: C10H17NO3
SMILES: CN1C2CCC1CC(OC(=O)CO)C2
Mol. weight [g/mol]: 199.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.83		Crippen Method
logp	0.147		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
rinsol	1420.00		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=R421606&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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