6-Hydroxyacetoxytropane

Inchi: InChI=1S/C10H17NO3/c1-11-7-3-2-4-8(11)9(5-7)14-10(13)6-12/h7-9,12H,2-6H2,1H3/t7-,
InchiKey: XIYRPSDQEWSIRW-YIZRAAEISA-N
Formula: C10H17NO3
SMILES: CN1C2CCCC1C(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
rinpol	1438.00		NIST Webbook
rinpol	1438.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R421735&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.