

6-Acetoxytropan-3-ol

Inchi:	InChI=1S/C10H17NO3/c1-6(12)14-10-4-7-3-8(13)5-9(10)11(7)2/h7-10,13H,3-5H2,1-2H3
InchiKey:	AEVQETQLKSVJET-UHFFFAOYSA-N
Formula:	C10H17NO3
SMILES:	CC(=O)OC1CC2CC(O)CC1N2C
Mol. weight [g/mol]:	199.25
CAS:	112546-76-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.94		Crippen Method
logp	0.146		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
rinpol	1500.00		NIST Webbook
rinpol	1561.30		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112546766&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

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