3-Hydroxy-6-Tigloyloxytropane

Inchi:	InChI=1S/C13H21NO3/c1-4-8(2)13(16)17-12-6-9-5-10(15)7-11(12)14(9)3/h4,9-12,15H,5-
InchiKey:	FSTVJNLNEVDORU-XBXARRHUSA-N
Formula:	C13H21NO3
SMILES:	CC=C(C)C(=O)OC1CC2CC(O)CC1N2C
Mol. weight [g/mol]:	239.31
CAS:	110024-55-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.05		Crippen Method
logp	1.092		Crippen Method
mcvol	191.300	ml/mol	McGowan Method
rinpol	1836.00		NIST Webbook
rinpol	1905.80		NIST Webbook
rinpol	1839.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C110024550&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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