3-Tigloyloxy-6-propionyloxy-7-hydroxytropane

Inchi:	InChI=1S/C16H25NO5/c1-5-9(3)16(20)21-10-7-11-14(19)15(22-13(18)6-2)12(8-10)17(11
InchiKey:	HGOLJZZEGFBRMR-WEVVVXLNSA-N
Formula:	C16H25NO5
SMILES:	CC=C(C)C(=O)OC1CC2C(O)C(OC(=O)CC)C(C1)N2C
Mol. weight [g/mol]:	311.37
CAS:	872205-33-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.28		Crippen Method
logp	1.023		Crippen Method
mcvol	241.010	ml/mol	McGowan Method
rinpol	1985.80		NIST Webbook
rinpol	1985.80		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=C872205339&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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