

3«alpha»-Tigloyloxy-7«beta»-isobutyryloxytropan

Inchi:	InChI=1S/C17H27NO4/c1-6-11(4)17(20)21-13-7-12-8-15(14(9-13)18(12)5)22-16(19)10(2
InchiKey:	ADNCMUUXIVQCLS-JCQAAVPFSA-N
Formula:	C17H27NO4
SMILES:	CC=C(C)C(=O)OC1CC2CC(OC(=O)C(C)C)C(C1)N2C
Mol. weight [g/mol]:	309.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.08		Crippen Method
logp	2.299		Crippen Method
mcvol	249.230	ml/mol	McGowan Method
rinpola	2062.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R421468&Units=SI

Legend

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

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