3-Tigloyloxy-6-(2-Methylpropanoyl)oxy-7-hydroxy

Inchi:	InChI=1S/C17H27NO5/c1-6-10(4)17(21)22-11-7-12-14(19)15(13(8-11)18(12)5)23-16(20)
InchiKey:	RZKWUOOSGIFSGP-UXBLZVDNSA-N
Formula:	C17H27NO5
SMILES:	CC=C(C)C(=O)OC1CC2C(O)C(OC(=O)C(C)C)C(C1)N2C
Mol. weight [g/mol]:	325.40
CAS:	1341219-31-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.46		Crippen Method
logp	1.269		Crippen Method
mcvol	255.100	ml/mol	McGowan Method
rinpol	2208.10		NIST Webbook
rinpol	2208.10		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=C1341219315&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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