3,7-Dihydroxy-6-tigloyloxytropane

Inchi:	InChI=1S/C12H19NO4/c1-3-7(2)12(16)17-8-4-9-11(15)10(5-8)13(9)6-14/h3,8-11,14-15H
InchiKey:	WTNSOAMJOANJTH-XVNBXDOJSA-N
Formula:	C12H19NO4
SMILES:	CC=C(C)C(=O)OC1CC2C(O)C(C1)N2CO
Mol. weight [g/mol]:	241.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.39		Crippen Method
logp	0.022		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
rinpol	1955.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R421379&Units=SI
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

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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