

# 3-Tigloyloxy-6-(2-methylbutyryloxy)-tropane

**Inchi:** InChI=1S/C18H29NO4/c1-6-11(3)17(20)22-14-8-13-9-16(15(10-14)19(13)5)23-18(21)12  
**InchiKey:** LWJJYAYQOTXATC-IZZDOVSWSA-N  
**Formula:** C18H29NO4  
**SMILES:** CC=C(C)C(=O)OC1CC2CC(OC(=O)C(C)CC)C(C1)N2C  
**Mol. weight [g/mol]:** 323.43  
**CAS:** 39972-72-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.50		Crippen Method
logp	2.689		Crippen Method
mcvol	263.320	ml/mol	McGowan Method
rinpol	2475.30		NIST Webbook
rinpol	2093.00		NIST Webbook
rinpol	2093.00		NIST Webbook
rinpol	2475.30		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C39972720&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

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

Latest version available from:

<https://www.cheméo.com/cid/97-627-9/3-Tigloyloxy-6-2-methylbutyryloxy-tropane.pdf>

Generated by Cheméo on 2024-04-19 18:22:11.369657848 +0000 UTC m=+15840180.290235169.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.