3«alpha»,6«beta»-Ditigloyloxytropane

Inchi: InChI=1S/C18H27NO4/c1-6-11(3)17(20)22-14-8-13-9-16(15(10-14)19(13)5)23-18(21)12(
InchiKey: MJJVORBCNQQRMU-AVNBRKTCSA-N
Formula: C18H27NO4
SMILES: CC=C(C)C(=O)OC1CC2CC(OC(=O)C(C)=CC)C(C1)N2C
Mol. weight [g/mol]: 321.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.60		Crippen Method
logp	2.609		Crippen Method
mcvol	259.020	ml/mol	McGowan Method
rinpol	2141.00		NIST Webbook
rinpol	2220.00		NIST Webbook
rinpol	2141.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R411095&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: 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