

3,6-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-GNXRPPCSSA-N
Formula: C18H27NO4
SMILES: CC=C(C)C(=O)OC1CC2CC(OC(=O)C(C)=CC)C(C1)N2C
Mol. weight [g/mol]: 321.41
CAS: 47295-99-8

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	2587.30		NIST Webbook
rinpol	2587.30		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C47295998&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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

Latest version available from:

<https://www.chemeo.com/cid/99-500-7/3-6-Ditigloyloxytropane.pdf>

Generated by Cheméo on 2024-04-27 09:26:50.188441464 +0000 UTC m=+16499259.109018779.

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