

7,9-Ditigloylplatynecine

Inchi: InChI=1S/C18H27NO4/c1-5-12(3)17(20)22-11-14-7-9-19-10-8-15(16(14)19)23-18(21)13
InchiKey: XNVWZRLIZINRQU-IUPTZTBESA-N
Formula: C18H27NO4
SMILES: CC=C(C)C(=O)OCC1CCN2CCC(OC(=O)C(C)=CC)C12
Mol. weight [g/mol]: 321.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.13		Crippen Method
logp	2.468		Crippen Method
mcvol	259.020	ml/mol	McGowan Method
rinpol	2252.00		NIST Webbook
rinpol	2300.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R177978&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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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