3«alpha»-Methylitaconyloxy-6«beta»-angeloyloxy

Inchi: InChI=1S/C19H27NO6/c1-6-11(2)18(22)26-16-9-13-8-14(10-15(16)20(13)4)25-19(23)12(
InchiKey: VPBVBTZJSHOYBI-HJLHVWOGSA-N
Formula: C19H27NO6
SMILES: C=C(CC(=O)OC)C(=O)OC1CC2CC(OC(=O)C(C)=CC)C(C1)N2C
Mol. weight [g/mol]: 365.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.88		Crippen Method
logp	1.762		Crippen Method
mcvol	280.550	ml/mol	McGowan Method
rinpol	2401.00		NIST Webbook
rinpol	2401.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R570055&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

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