7-Tigloyl-9-dihydroxysenecioylretronecine

Inchi: InChI=1S/C18H27NO6/c1-5-11(2)16(21)25-13-7-9-19-8-6-12(14(13)19)10-24-17(22)15(2
InchiKey: OSBDGPXHJXTOQT-HBTYBXAFSA-N
Formula: C18H27NO6
SMILES: CC=C(C)C(=O)OC1CCN2CC=C(COC(=O)C(O)C(C)(C)O)C12
Mol. weight [g/mol]: 353.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.12		Crippen Method
logp	0.554		Crippen Method
mcvol	270.760	ml/mol	McGowan Method
rinpol	2420.00		NIST Webbook
rinpol	2420.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R405248&Units=SI

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.