7-Hydroxyisovaleroyl-9-viridifloryl-retronecine

Inchi: InChI=1S/C20H33NO7/c1-12(2)20(26,13(3)22)18(24)27-11-14-6-8-21-9-7-15(17(14)21)2
InchiKey: COXZBOZLTKZNDP-QWQDWOJRSA-N
Formula: C20H33NO7
SMILES: CC(C)C(O)(C(=O)OCC1=CCN2CCC(OC(=O)CC(C)(C)O)C12)C(C)O
Mol. weight [g/mol]: 399.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	0.385		Crippen Method
mcvol	309.110	ml/mol	McGowan Method
rinpol	2569.00		NIST Webbook
rinpol	2569.00		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=R335243&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.