dihydroxytriangularicine

Inchi: InChI=1S/C18H27NO7/c1-4-11(2)16(22)26-14-6-8-19-7-5-13(15(14)19)9-25-17(23)18(24
InchiKey: IMZYUCHNYPUYBN-GJMSLPJUSA-N
Formula: C18H27NO7
SMILES: CC=C(C)C(=O)OC1CCN2CC=C(COC(=O)C(O)(CO)C(C)O)C12
Mol. weight [g/mol]: 369.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.39		Crippen Method
logp	-0.474		Crippen Method
mcvol	276.630	ml/mol	McGowan Method
rinpol	2550.00		NIST Webbook

Sources

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=R227979&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices