

dihydroxytriangularine

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-LJTWXBORSA-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
rinsol	2525.00		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=R227984&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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<https://www.chemeo.com/cid/32-432-6/dihydroxytriangularine.pdf>

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