Heliosupine

Other names:	2-Butenoic acid, 2-methyl-, 7-[[2,3-dihydroxy-2-(1-hydroxyethyl)-3-methyl-1-oxobutoxy]methyl]-2,3,5,7a-tetrahydro-1H ester
	Cynoglossofin
	Cynoglossofine
	Cynoglossophine
	Heliosupin
Inchi:	InChI=1S/C20H31NO7/c1-6-12(2)17(23)28-15-8-10-21-9-7-14(16(15)21)11-27-18(24)20(
InchiKey:	HRSGCYGUWHGOPY-PUYHTSCPSA-N
Formula:	C20H31NO7
SMILES:	CC=C(C)C(=O)OC1CCN2CC=C(COC(=O)C(O)(C(C)O)C(C)(C)O)C12
Mol. weight [g/mol]:	397.46
CAS:	32728-78-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.34		Crippen Method
logp	0.305		Crippen Method
mcvol	304.810	ml/mol	McGowan Method
rinpol	2555.00		NIST Webbook
rinpol	2553.00		NIST Webbook
rinpol	2550.00		NIST Webbook
rinpol	2555.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32728782&Units=SI
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

Legend

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

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https://www.chemeo.com/cid/11-280-8/Heliosupine.pdf

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