[1R-(1«alpha»,7a«beta»)]-[1-((Z)-2-Methyl-1-oxobu
ester of (Z)-2-hydroxymethylbut-2-enoic acid

Othernames: Alkaloid A
2-Butenoic acid, 2-(hydroxymethyl)-, [2,3,5,7a-tetrahydro-1-[(2-methyl-1-oxo-2-butenyl)oxy]-1H-pyrrolizin-7-yl]methyl ester, [1R-[1«alpha»(Z),7(Z),7a«beta»]]-
Triangularine

Inchi: InChI=1S/C18H25NO5/c1-4-12(3)17(21)24-15-7-9-19-8-6-14(16(15)19)11-23-18(22)13(5

InchiKey: GOENJWUGVSLZDQ-JBWWEBJPSA-N

Formula: C18H25NO5

SMILES: CC=C(C)C(=O)OC1CCN2CC=C(COC(=O)C(=CC)CO)C12

Mol. weight [g/mol]: 335.39

CAS: 87340-27-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.49		Crippen Method
logp	1.361		Crippen Method
mcvol	260.590	ml/mol	McGowan Method
rinpol	2375.00		NIST Webbook
rinpol	2375.00		NIST Webbook
rinpol	2375.00		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=C87340270&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