Butanoic acid, 2,3-dihydroxy-2-(1-methylethyl)-, (2,3,5,7a-tetrahydro-1-hydroxy-1H-pyrrolizin-7-yl)m ester, [1S-[1«alpha»,7(2R*,3R*),7a«alpha»]]-

Other names:	Echimatine
Iupac:	Butanoic acid, 2,3-dihydroxy-2-(1-methylethyl)-, (2,3,5,7a-tetrahydro-1-hydroxy-1H-pyrrolizin-7-yl)methyl ester, [1S-[1«alpha»,7(2R*,3R*),7a«alpha»]]-
InchiKey:	SFVVQRJOGUKCEG-UHFFFAOYSA-N
Formula:	C15H25NO5
SMILES:	CC(C)C(O)(C(=O)OCC1=CCN2CCC(O)C12)C(C)O
Mol. weight [g/mol]:	299.36
CAS:	480-83-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.17		Crippen Method
logp	-0.327		Crippen Method
mcvol	231.220	ml/mol	McGowan Method
rinpol	2170.00		NIST Webbook
rinpol	2175.00		NIST Webbook
rinpol	2172.00		NIST Webbook
rinpol	2172.00		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=C480831&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