2-Butenoic acid, 2-methyl-, 2,3,5,7a-tetrahydro-7-(hydroxymethyl)-1H-pyrroliz ester, [1S-[1«alpha»(Z),7a«alpha»]]-

Othernames: Heliotridine 7-(2-methylcrotonate), (Z)-
Heliotridine, 7-angelate (ester)
Rivularine
Heliotridine, 7-angelyl-
7-Angeloylheliotridine
7-Angelylheliotridine
7-(Hydroxymethyl)-(1S,7aR)-2,3,5,7a-tetrahydro-1H-pyrrolizin-1-yl (2Z)-2-methyl-2-butenoate
Heliotridine, 7-angelate

Inchi: InChI=1S/C13H19NO3/c1-3-9(2)13(16)17-11-5-7-14-6-4-10(8-15)12(11)14/h3-4,11-12,15

InchiKey: TYGYPIIOOQNWBU-YKSZOPSQSA-N

Formula: C13H19NO3

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

Mol. weight [g/mol]: 237.29

CAS: 723-78-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.68		Crippen Method
logp	0.871		Crippen Method
mcvol	187.000	ml/mol	McGowan Method
rinpol	1820.00		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1821.00		NIST Webbook
rinpol	1818.00		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1818.00		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1820.00		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=C723784&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