

[1R-(1 «alpha»,7a «beta»)]-[1-((Z)-2-Methyl-1-oxobut-2-enyl)]-1H-pyrrolizine-7-yl methyl ester of (Z)-2-hydroxymethylbut-2-enoic acid

Other names:

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»]]-triangular

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/ci9903071>

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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