



CAS Registry Number: 211944-25-1

Molecular Formula: C₄₂H₆₈O₁₆

Molecular Weight: 828.99

Accurate Mass: 828.45074

Percentage Composition: C 60.85%; H 8.27%; O 30.88%

Biological Source: Constit. of *Acorus calamus*

Physical Description: Cryst. (CHCl₃)

Melting Point: Mp 94°

>> **Derivative:** Me ester

CAS Registry Number: 263706-07-6

Molecular Formula: C₃₁H₅₀O₆

Molecular Weight: 518.732

Accurate Mass: 518.36074

Percentage Composition: C 71.78%; H 9.72%; O 18.51%

Biological Source: Constit. of *Centipeda minima*

>> **Derivative:** 2-Ketone

Synonym(s): 1,3,19-Trihydroxy-2-oxo-12-ursen-28-oic acid. 1-Hydroxy-2-oxopomolic acid

CAS Registry Number: 217466-37-0

Molecular Formula: C₃₀H₄₆O₆

Molecular Weight: 502.69

Accurate Mass: 502.32944

Percentage Composition: C 71.68%; H 9.22%; O 19.10%

Biological Source: Constit. of *Rosa woodsii*

Physical Description: Cryst. (Et₂O/hexane)

Melting Point: Mp 227-229°

Optical Rotation: [α]_D²³ -105.6 (c, 0.26 in MeOH)

>> **Variant:** (1 β ,2 β ,3 β ,19 α)-form

Molecular Formula: C₃₀H₄₈O₆

Molecular Weight: 504.706

Accurate Mass: 504.34509

Percentage Composition: C 71.39%; H 9.59%; O 19.02%

Biological Source: Constit. of *Agrimonia pilosa*

>> **Derivative:** Me ester

CAS Registry Number: 263706-08-7

Molecular Formula: C₃₁H₅₀O₆

Molecular Weight: 518.732

Accurate Mass: 518.36074

Percentage Composition: C 71.78%; H 9.72%; O 18.51%

Biological Source: Constit. of *Centipeda minima*

References:

- Kouno, I. *et al.*, *Phytochemistry*, 1988, **27**, 297
Guang-Yi, L. *et al.*, *J. Nat. Prod.*, 1989, **52**, 162, (*isol, pmr, cmr*)
Srivastava, M. *et al.*, *Int. J. Pharmacogn.*, 1994, **32**, 197, (*glucosyl ester*)
Rai, R. *et al.*, *Indian J. Chem., Sect. B*, 1998, **37**, 473-476, (*Acorus calamus saponin*)
Kashiwada, Y. *et al.*, *J. Nat. Prod.*, 1998, **61**, 1090-1095, (*1 β -Hydroxy-2-oxopomolic acid*)
Li, B.-Z. *et al.*, *Phytochemistry*, 1998, **49**, 2477-2481, (*1 α ,2 α ,3 β ,19 α -form*)
Rai, N. *et al.*, *Pharm. Biol.*, 1999, **37**, 314-317, (*Me esters*)
Mei, W.L. *et al.*, *Chin. Chem. Lett.*, 2000, **11**, 1013-1014, (*Dichotomanthes tristaniaecarpa constit*)