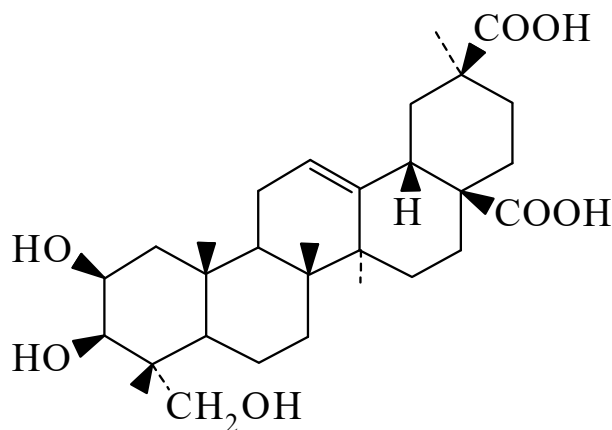




>>Entry Name: 2,3,23-Trihydroxy-12-oleanene-28,30-dioic acid



Molecular Formula: C₃₀H₄₆O₇

Molecular Weight: 518.689

Accurate Mass: 518.324355

Percentage Composition: C 69.47%; H 8.94%; O 21.59%

>>Variant: (2β,3β)-form

Synonym(s): Jaligonic acid. Desmethylphytolaccagenin

CAS Registry Number: 51776-39-7

Molecular Formula: C₃₀H₄₆O₇

Molecular Weight: 518.689

Accurate Mass: 518.324355

Percentage Composition: C 69.47%; H 8.94%; O 21.59%

Use/Importance: Antiinflammatory agent, diuretic

Physical Description: Cryst. (MeOH)

Melting Point: Mp 315-325 dec.° (318-320°)

Calculated Log P Data: Log P 3.29 (calc)

>>Derivative: 30-Me ester

Synonym(s): Phytolaccagenin

CAS Registry Number: 1802-12-6

Molecular Formula: C₃₁H₄₈O₇

Molecular Weight: 532.716

Accurate Mass: 532.340005

Percentage Composition: C 69.89%; H 9.08%; O 21.02%

Biological Source: Aglycone from *Phytolacca* spp.

Use/Importance: Possesses antiinflammatory props.

Physical Description: Cryst. (MeOH)

Melting Point: Mp 317-318 dec.°

Optical Rotation: [α]_D²⁶+113.7 (c, 0.89 in MeOH)

Solubility: BERDY SOL: Sol. MeOH, Py

Calculated Log P Data: Log P 3.71 (calc)

>>Derivative: 3-Ac, 30-Me ester

Synonym(s): Phytolaccagenin A

CAS Registry Number: 95260-99-4

Molecular Formula: C₃₃H₅₀O₈

Molecular Weight: 574.753

Accurate Mass: 574.35057

Percentage Composition: C 68.96%; H 8.77%; O 22.27%

Biological Source: Constit. of *Phytolacca acinosa*

Physical Description: Cryst.

Melting Point: Mp 165°