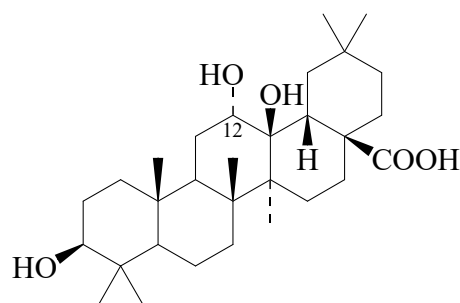




>>Entry Name: 3,12,13-Trihydroxy-28-oleananoic acid



(3 $\beta$ ,12 $\alpha$ ,13 $\beta$ )-form

Related CAS Registry Numbers(s): 74048-38-7

Molecular Formula: C<sub>30</sub>H<sub>50</sub>O<sub>5</sub>

Molecular Weight: 490.722

Accurate Mass: 490.365825

Percentage Composition: C 73.43%; H 10.27%; O 16.30%

>>Variant: (3 $\beta$ ,12 $\alpha$ ,13 $\beta$ )-form

Molecular Formula: C<sub>30</sub>H<sub>50</sub>O<sub>5</sub>

Molecular Weight: 490.722

Accurate Mass: 490.365825

Percentage Composition: C 73.43%; H 10.27%; O 16.30%

>>Derivative: 28→13 Lactone

Synonym(s): 3,12-Dihydroxy-28,13-oleananolide

Molecular Formula: C<sub>30</sub>H<sub>48</sub>O<sub>4</sub>

Molecular Weight: 472.707

Accurate Mass: 472.35526

Percentage Composition: C 76.23%; H 10.23%; O 13.54%

>>Derivative: 28→13 Lactone, 3-Ac

CAS Registry Number: 62498-83-3

Molecular Formula: C<sub>32</sub>H<sub>50</sub>O<sub>5</sub>

Molecular Weight: 514.744

Accurate Mass: 514.365825

Percentage Composition: C 74.67%; H 9.79%; O 15.54%

Biological Source: Constit. of *Rhodomyrtus tomentosa* and *Pieris japonica*

Physical Description: Cryst.

Melting Point: Mp 301-303° (284-286°)

Optical Rotation: [ $\alpha$ ]<sub>D</sub> +39.7 (CHCl<sub>3</sub>)

Other Data: Initially descr. in CA as an ursane

>>Derivative: 28→13 Lactone, 3-O-[ $\beta$ -D-xylopyranosyl-(1→3)- $\beta$ -D-glucuronopyranoside]

Synonym(s): Kochianoside III

Molecular Formula: C<sub>41</sub>H<sub>64</sub>O<sub>14</sub>

Molecular Weight: 780.948

Accurate Mass: 780.42961

Percentage Composition: C 63.06%; H 8.26%; O 28.68%

Biological Source: Constit. of *Kochia scoparia*

Physical Description: Cryst. (CHCl<sub>3</sub>/MeOH)

Melting Point: Mp 224-225°

Optical Rotation: [ $\alpha$ ]<sub>D</sub><sup>26</sup> +47.9 (c, 0.6 in MeOH)