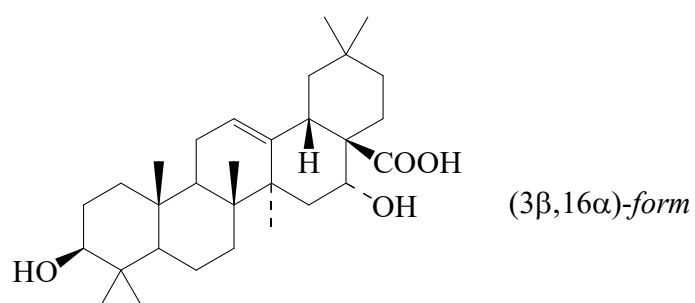




>>Entry Name: 3,16-Dihydroxy-12-oleanen-28-oic acid



Related CAS Registry Number(s): 69280-20-2

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%

>>Variant: (3β,16α)-form

Synonym(s): Echinocystic acid. Albizziagenin

CAS Registry Number: 510-30-5

Type of Compound Code(s): XA4150 XA0900 VS8300

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%

Biological Source: Sapogenin from *Echinocystis* spp., *Albizzia* spp. and others

Biological Use/Importance: Anthelmintic. Possesses expectorant props.

Physical Description: Cryst. (EtOH)

Melting Point: Mp 305-312 dec.°

Optical Rotation:  $[\alpha]_D^{26} +27.7$  (EtOH)

Calculated Log P Data: Log P 7.21 (uncertain value) (calc)

>>Derivative: Me ester

CAS Registry Number: 2309-45-7

Molecular Formula: C<sub>31</sub>H<sub>50</sub>O<sub>4</sub>

Molecular Weight: 486.734

Percentage Composition: C 76.50%; H 10.35%; O 13.15%

Melting Point: Mp 211-213°

>>Derivative: 3-O-Sulfate

Type of Compound Code(s): VS8300

Molecular Formula: C<sub>30</sub>H<sub>48</sub>O<sub>7</sub>S

Molecular Weight: 552.771

Accurate Mass: 552.312075

Percentage Composition: C 65.19%; H 8.75%; O 20.26%; S 5.80%

Biological Source: Constit. of *Tetrapleura tetraptera*

Physical Description: Powder (MeOH aq.)

Melting Point: Mp 194-197°

>>Derivative: 28-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl] ester, 3-O-sulfate

Synonym(s): Rotundioside A

CAS Registry Number: 99633-17-7

Type of Compound Code(s): VS8300

Molecular Formula: C<sub>54</sub>H<sub>88</sub>O<sub>27</sub>S

Molecular Weight: 1201.339

Accurate Mass: 1200.523375

Percentage Composition: C 53.99%; H 7.38%; O 35.96%; S 2.67%

Biological Source: Isol. from leaves of *Bupleurum rotundifolium*

Melting Point: Mp 232-237°

Optical Rotation:  $[\alpha]_D^{23} -11.6$  (c, 0.78 in MeOH)