



Formula: C₃₀H₄₈O₃

MW: 456.71

CAS: 508-02-1

MDL: MFCD03225497

TNP: TNP00102

(3-β)-3-hydroxyolean-12-en-28-oic acid; (3-β)-olean-12-en-28-oic acid;
(3β)-olean-12-en-28-oic acid; 3-β-hydroxy-olean-12-en-28-oic acid; astrantiagenin;
giganteumgenin; virgaureagenin; CARYOPHYLLIN



LogP: 1.74

LogS: -3.3

Acceptors: 3

Donors: 2

Rotation Bonds: 1

Chiral Centers: 8

N+O: 3

LIPINSKY: 4

IUPAC: (2S,5S,10S,18S,1R,14R,15R,20R)-18-hydroxy-1,2,8,8,15,19,19-heptamethylpentacyclop[12.8.0.0.0.0]docos-11-ene-5-carboxylic acid

Smiles:

C1=2[C]([C]3([C@@H]([C]4(CC[C@@H](C([C@@H]4(CC3)))(C)C)O)C)CC2C)(CC[C@@]2(C(=O)O)CCC(C[C@@H]12)(C)C)C

Specification: Pentacyclic triterpenes; Tri-Terpenoids; Biochemistry; Terpenes; Terpenes (Others); Natural Plant Extract; Anti-proliferative Agents Asymmetric Synthesis; Complex Molecules Nutrition Research; Isoprenoid/terpenoid Cancer Research; Phase I Enzyme Inhibitors; Phase I Enzyme Inhibitors Cancer Research; Biochemicals Found in Plants; Cancer Research; Chemopreventive Agents; Chiral Building Blocks; Multidrug Resistance Oleanic acid Chemical Properties:

mp >300 C(lit.) storage temp. 2-8C color light yellow Merck 6827 CAS DataBase Reference 508-02-1 (CAS DataBase Reference) EPA Substance Registry System Olean-12-en-28-oic acid, 3-hydroxy-, (3.beta.)-(508-02-1) Safety Information Hazard Codes Xi Risk Statements 36/37/38 Safety Statements 26-36-37/39 WGK Germany 2 RTECS RK0177965 3beta-Hydroxyolean-12-en-28-oic acid English Oleanic acid Usage And Synthesis Oleanic acid

Merck 13 Reference: Monograph Number: 0006897

Title: Oleanolic Acid

CAS Registry Number: 508-02-1

CAS Name: (3b)-3-Hydroxyolean-12-en-28-oic acid

Additional Names: oleanol; caryophyllin

Molecular Formula: C₃₀H₄₈O₃

Molecular Weight: 456.70.

Percent Composition: C 78.90%, H 10.59%, O 10.51%

Literature References: Occurs in the free state in leaves of *Olea europaea*, Oleaceae, in leaves of *Viscum album* L., Loranthaceae, in buds of *Syzygium aromaticum* (L.) Merr. & Perry, Myrtaceae (cloves), in *Swertia japonica* (Maxim.) Makino, and in *Centaureum umbellatum* Gilib. (*Erythraea centaureum* (L.) Pers.), Gentianaceae; as acetate in birch bark, as glycoside in many saponins. Isoln procedures (from cloves): Winterstein, Stein, Z. Physiol. Chem. 202, 222 (1931); Ruzicka, Hofmann, Helv. Chim. Acta 19, 114 (1936); Picard et al., J. Chem. Soc. 1939, 1047. Structure: Ruzicka et al., Helv. Chim. Acta 29, 210 (1946). Review: J. Simonsen, W. C. T. Ross, The Terpenes vol. 5 (University Press, Cambridge, 1957) pp 221-285. Cf. a- and b-amyrin.

Properties: Fine, solvated needles from alc. After drying, mp 310. [α]_D²⁰ +83.3 (c = 0.6 in chloroform). pK 2.52. Insol in water. Sol in 65 parts ether, 106 parts 95% alcohol, 35 parts boiling 95% alcohol, 118 parts chloroform, 180 parts acetone, 235 parts methanol.

Melting point: mp 310

pKa: pK 2.52

Optical Rotation: $[\alpha]_{D20} +83.3$ (c = 0.6 in chloroform)

Derivative Type: Acetate

Molecular Formula: C₃₂H₅₀O₄

Molecular Weight: 498.74.

Percent Composition: C 77.06%, H 10.10%, O 12.83%

Properties: Needles from methanol, mp 268. $[\alpha]_{D17} +74.5$ (c = 0.6 in CHCl₃).

Melting point: mp 268

Optical Rotation: $[\alpha]_{D17} +74.5$ (c = 0.6 in CHCl₃)

Derivative Type: Methyl ester

Molecular Formula: C₃₁H₅₀O₃

Molecular Weight: 470.73.

Percent Composition: C 79.10%, H 10.71%, O 10.20%

Properties: mp 201. $[\alpha]_{D20} +75$ (c = 0.6 in CHCl₃).

Melting point: mp 201

Optical Rotation: $[\alpha]_{D20} +75$ (c = 0.6 in CHCl₃)

Derivative Type: Acetate of methyl ester

Molecular Formula: C₃₃H₅₂O₄

Molecular Weight: 512.76.

Percent Composition: C 77.30%, H 10.22%, O 12.48%

Properties: Needles from alcohol, mp 223. $[\alpha]_{D20} +70$ (c = 0.6 in CHCl₃).

Melting point: mp 223

Optical Rotation: $[\alpha]_{D20} +70$ (c = 0.6 in CHCl₃)