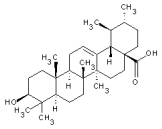

Formula: C30H48O3

MW: 456.71

CAS: 77-52-1

MDL: MFCD03225446

TNP: TNP00103

LogP: 5.33

LogS: -5.23

Acceptors: 3

Donors: 2

Rotation Bonds: 1

Chiral Centers: 10

N+O: 3

LIPINSKY: 4

IUPAC: (2S,5S,9S,10S,18S,1R,8R,14R,15R,20R)-18-hydroxy-1,2,8,9,15,19,19-heptamethylpentacyclo[12.8.0.0.0.0]docos-11-ene-5-carboxylic acid

Smiles:
C1=2[C]([C]3(CC[C@@H]4([C]([C@H]3(CC2))(CC[C@@H](O)C4(C)C)C))C)(CC[C]2([C@H]1([C@H]([C@@H](CC2)C)C))C(=O)O)C

Merck 13 Reference: Monograph Number: 0009957

Title: Ursolic Acid

CAS Registry Number: 77-52-1

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

Additional Names: urson; prunol; micromerol; malol

Molecular Formula: C30H48O3

Molecular Weight: 456.70.

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

Literature References: In leaves and berries of Arctostaphylos uva-ursi (L.) Spreng (bearberry), of Vaccinium macrocarpon Ait. (cranberry), Rhododendron hymenanthes Makino, Ericaceae. In the protective wax-like coating of apples, pears, prunes, and other fruits. Isoln from apple peelings: Sando, J. Biol. Chem. 56, 457 (1923). Structure: Ruzicka et al., Helv. Chim. Acta 28, 199 (1945); Zurcher et al., ibid. 37, 2145 (1954). Conversion from a-amyrin: Boar et al., J. Chem. Soc. C 1970, 678. Chemistry: Mezzetti et al., Planta Med. 20, 244 (1971).

Properties: Large, lustrous prisms from abs alcohol, fine hair-like needles from dil alcohol, mp 285-288. [a]D21 +67.5 (c = 1 in N alc KOH). Soly at 15: One part dissolves in 88 parts methanol, 178 alcohol (35 boiling alcohol), 140 ether, 388 chloroform, 1675 carbon disulfide. Moderately sol in acetone. Sol in hot glacial acetic acid and in 2% alcoholic NaOH. Insol in water and petr ether.

Melting point: mp 285-288

Optical Rotation: [a]D21 +67.5 (c = 1 in N alc KOH)

Derivative Type: Acetate

Molecular Formula: C32H50O4

Molecular Weight: 498.74.

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

Properties: mp 289-290. [a]D +62.3 (c = 1.15 in chloroform).

Melting point: mp 289-290

Optical Rotation: [a]D +62.3 (c = 1.15 in chloroform)

Derivative Type: Methyl ester

Molecular Formula: C31H50O3

Molecular Weight: 470.73.

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

Properties: mp 171. [a]D20 +58 (c = 1.2 in pyridine).

Melting point: mp 171

Optical Rotation: [a]D20 +58 (c = 1.2 in pyridine)

Derivative Type: Methyl ester acetate

Molecular Formula: C33H52O4

Molecular Weight: 512.76.

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

Properties: mp 246-247.

Melting point: mp 246-247

Use: As emulsifying agent in pharmaceuticals, foods.