



Formula: C<sub>48</sub>H<sub>78</sub>O<sub>19</sub>

MW: 959.14

CAS: 16830-15-2

Smiles:

C1C2C(CC(C(C2(CO)C)O)O)(C2C(C1)(C1(C(=CC2)C2C(CC1)(CCC(C2C)C)C(OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)CO)OC1C(C(C(C(O1)C)O)O)O)O)=O)C)C)C

REFERENCE: [1] Anti-herpes simplex virus activities of crude water extracts of Thai medicinal plants: C. Yoosook, et al.; *Phytomedicine* 6, 411 (2000) [2] Glycoside-bearing liposomal delivery systems against macrophage-associated disorders involving *Mycobacterium leprae* and *Mycobacterium tuberculosis*: S. Medda, et al.; *Indian. J. Biochem. Biophys.* 32, 147 (1995) [3] In vitro and in vivo wound healing activity of asiaticoside isolated from *Centella asiatica*: A. Shukla, et al.; *J Ethnopharmacol* 65, 1 (1999) [4] Triterpenes from *Centella asiatica* stimulate extracellular matrix accumulation in rat experimental wounds: F.X. Maquart, et al.; *Eur. J. Dermatol.* 9, 289 (1999) [5] Protective effects of asiaticoside derivatives against beta-amyloid neurotoxicity: I. Mook-Jung, et al.; *J. Neurosci. Res.* 58, 417 (1999)

SOURCE: Asiaticoside is a triterpene glycoside from the plant *Centella asiatica*, commonly used in wound healing. This activity is a result of stimulation of collagen and glycosaminoglycan synthesis [1,2]. This glycoside was also found to have activity against her

ACCEPTORS: 19

DONORS: 12

ROTATION BONDS: 22

N+O: 19

Chiral Centers: 27

LogP: 0.1

LogS: -5.71

LIPINSKI: 1

Synonyms:

2-alpha,3-beta,23-trihydroxy-urs-12-en-28-oicacio-6-deoxy-alpha-l-mannopy;asiaticosid;blastoe  
stimulina;dermatologico;ranosyl-(1-4)-o-beta-d-glucopyranosyl-(1-6)-o-beta-d-glucopyranosylest  
er;[6-[[[3,4-Dihydroxy-6-(hydroxymethyl)-5-(3,4,5-trihydroxy-6-methyl-oxan-2-yl)oxy-oxan-2-yl]ox  
ymethyl]-3,4,5-trihydroxy-oxan-2-yl]  
(1S,2R,4aS,6aS,6bR,9S,10R,11R,12aS,14bR)-10,11-dihydroxy-9-(hydroxymethyl)-1,2,6a,6b,9,  
12a-hexamethyl-2,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydro-1H-picene-4a-carboxylate;  
CENTELASE;ASIATICOSIDE

CAS:16830-15-2

MF:C48H78O19

MW:959.12

EINECS:240-851-7

Product Categories:Saponins;Alkaloids;Natural Plant Extract;The group of Asiaticoside  
Asiaticoside

Chemical Properties: mp 235-238C

CAS DataBase Reference: 16830-15-2(

CAS DataBase Reference: )

Safety Information: WGK Germany 3 RTECS YU9625000 F 1-10

[6-[[[3,4-Dihydroxy-6-(hydroxymethyl)-5-(3,4,5-trihydroxy-6-methyl-oxan-2-yl)oxy-oxan-2-yl]oxym

ethyl]-3,4,5-trihydroxy-oxan-2-yl]

(1S,2R,4aS,6aS,6bR,9S,10R,11R,12aS,14bR)-10,11-dihydroxy-9-(hydroxymethyl)-1,2,6a,6b,9,12a-hexamethyl-2,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydro-1H-picene-4a-carboxylate  
Asiaticoside

Usage And Synthesis: Asiaticoside

