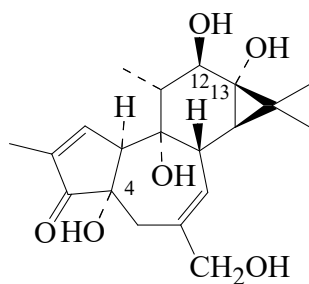




>>Entry Name: 4,9,12,13,20-Pentahydroxy-1,6-tigliadien-3-one



(4 α ,9 α ,12 β ,13 α)-form

Related CAS Registry Numbers(s): 16675-05-1 24928-15-2 24928-17-4 25405-85-0 37558-16-0 57716-89-9 61557-88-8 71295-86-8

Molecular Formula: C₂₀H₂₈O₆

Molecular Weight: 364.438

Accurate Mass: 364.18859

Percentage Composition: C 65.92%; H 7.74%; O 26.34%

>>Variant: (4 α ,9 α ,12 β ,13 α)-form

Synonym(s): Isophorbol. 4 α -Phorbol

CAS Registry Number: 26241-63-4

Molecular Formula: C₂₀H₂₈O₆

Molecular Weight: 364.438

Accurate Mass: 364.18859

Percentage Composition: C 65.92%; H 7.74%; O 26.34%

Biological Source: Constit. of croton oil

Physical Description: Hygroscopic cryst. (EtOAc)

Melting Point: Mp 135-150°

Sigma: P4888

>>Derivative: 12,13-Didecanoyl

CAS Registry Number: 27536-56-7

Molecular Formula: C₄₀H₆₄O₈

Molecular Weight: 672.941

Accurate Mass: 672.46012

Percentage Composition: C 71.39%; H 9.59%; O 19.02%

UV: [neutral] $\lambda_{\max}$ 207 (); 238 (); 334 () (no solvent reported)

>>Derivative: 12-O-(2-Methylaminobenzoyl), 13-Ac

CAS Registry Number: 82042-11-3

Molecular Formula: C₃₀H₃₇NO₈

Molecular Weight: 539.624

Accurate Mass: 539.251919

Percentage Composition: C 66.77%; H 6.91%; N 2.60%; O 23.72%

Biological Source: Constit. of *Sapium indicum*

>>Variant: (4 β ,9 α ,12 β ,13 α)-form

Synonym(s): Phorbol

CAS Registry Number: 17673-25-5

Molecular Formula: C₂₀H₂₈O₆

Molecular Weight: 364.438

Accurate Mass: 364.18859

Percentage Composition: C 65.92%; H 7.74%; O 26.34%

Biological Source: Produced by hydrol. of cocarcinogens from croton oil (*Croton tiglium*) and from *Sapium* and *Euphorbia* spp.

Physical Description: Cryst. + MeOH (MeOH)

Melting Point: Mp 240-250°. Mp 250-251 dec.° (solvent free)

Optical Rotation: $[\alpha]_{\text{D}}^{20} +118$ (c, 0.4 in dioxan)

Hazard & Toxicity: Skin irritant. Esters are potent tumour-promoting agents

Sigma: P8893