



Percentage Composition: C 54.54%; H 6.71%; O 38.75%

>>**Derivative:** 2-Octanoyl, 3-angeloyl, 8-butanoyl, 10-Ac

Synonym(s): Thapsigargin

CAS Registry Number: 67526-95-8

Molecular Formula: C₃₄H₅₀O₁₂

Molecular Weight: 650.762

Accurate Mass: 650.33023

Percentage Composition: C 62.75%; H 7.74%; O 29.50%

Biological Source: Constit. of *Thapsia garganica*

Biological Use/Importance: Inhibits intracellular Ca²⁺ transport ATPases. Mobilises intracellular Ca²⁺ stores. Pharmacol. tool for studying Ca²⁺ homeostasis. Induces apoptosis in a variety of cell lines. Histamine secretagogue

Other Data: The abs. config. is unprecedented and is presumably associated with the presence of the 7-OH group

Hazard & Toxicity: Skin irritant. Stimulates production of Histamine HJF38-X. Promotes tumourigenesis in mouse skin

Sigma: T9033

>>**Derivative:** 2-Hexanoyl, 3-angeloyl, 8-butanoyl, 10-Ac

Synonym(s): Thapsigargin. 7-Epicapitatin

CAS Registry Number: 67526-94-7

Molecular Formula: C₃₂H₄₆O₁₂

Molecular Weight: 622.708

Accurate Mass: 622.29893

Percentage Composition: C 61.72%; H 7.45%; O 30.83%

Biological Source: Constit. of *Thapsia garganica*

Biological Use/Importance: Inhibits sarcoplasmic reticulum Ca²⁺-ATPase

Physical Description: Gum

Solubility: BERDY SOL: Sol. MeOH, C₆H₆; poorly sol. H₂O

Hazard & Toxicity: Skin irritant

Sigma: T4557

>>**Variant:** (1 α ,2 α ,3 β ,6 α ,7 α OH,8 β ,10 α ,11 β)-form

Molecular Formula: C₁₅H₂₂O₈

Molecular Weight: 330.334

Accurate Mass: 330.13147

Percentage Composition: C 54.54%; H 6.71%; O 38.75%

>>**Derivative:** 2-(3-Methyl-2-butenoyl), 3-angeloyl, 8-(2-methylbutanoyl), 10-Ac

Synonym(s): Thapsivillosin K

CAS Registry Number: 99270-55-0

Molecular Formula: C₃₂H₄₄O₁₂

Molecular Weight: 620.692

Accurate Mass: 620.28328

Percentage Composition: C 61.92%; H 7.14%; O 30.93%

Biological Source: Constit. of *Thapsia villosa*

Physical Description: Cryst. (C₆H₆/hexane)

Melting Point: Mp 119-121°

Optical Rotation: [α]_D²⁵ -28.6 (c, 2.5 in CHCl₃)

Other Data: The abs. config. is likely to be the opposite of that indicated ie. same as those of Thapsigargin and Thapsigargin

References:

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