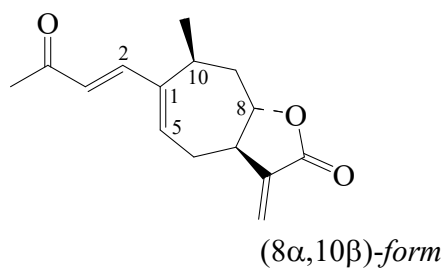




>>Entry Name: 4-Oxo-1(5),2,11(13)-xanthatrien-12,8-olide



Molecular Formula: C₁₅H₁₈O₃

Molecular Weight: 246.305

Accurate Mass: 246.125595

Percentage Composition: C 73.15%; H 7.37%; O 19.49%

>>Variant: (8 α ,10 β)-form

Synonym(s): Xanthatin

CAS Registry Number: 26791-73-1

Molecular Formula: C₁₅H₁₈O₃

Molecular Weight: 246.305

Accurate Mass: 246.125595

Percentage Composition: C 73.15%; H 7.37%; O 19.49%

Biological Source: Constit. of *Xanthium* spp.

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 114-115°

Optical Rotation: [α]_D -20

Solubility: BERDY SOL: Sol. MeOH, Et₂O; poorly sol. H₂O, bases, hexane

UV: [neutral] $\lambda_{\max}$ 284 () (MeOH) (Berdy) [neutral] $\lambda_{\max}$ 213 (ϵ 7300); 275 (ϵ 22800) (EtOH) (Berdy)

Hazard & Toxicity: BERDY HAZD : LD₅₀ (mus, ipr) 800 mg/kg

>>Derivative: 1 α ,5 α -Epoxide

Synonym(s): 1,5-Epoxy-4-oxo-2,11(13)-xanthadien-12,8 α -olide. 1 α ,5 α -Epoxyxanthatin

Molecular Formula: C₁₅H₁₈O₄

Molecular Weight: 262.305

Accurate Mass: 262.12051

Percentage Composition: C 68.69%; H 6.92%; O 24.40%

Biological Source: Constit. of *Xanthium spinosum*

Physical Description: Oil

>>Derivative: 1 β ,5 β -Epoxide

Synonym(s): 1 β ,5 β -Epoxyxanthatin

Molecular Formula: C₁₅H₁₈O₄

Molecular Weight: 262.305

Accurate Mass: 262.12051

Percentage Composition: C 68.69%; H 6.92%; O 24.40%

Biological Source: From *Xanthium spinosum*

Physical Description: Oil

>>Derivative: 2,3-Dihydro

Synonym(s): Xanthinosin. 8-Epitomentosin

CAS Registry Number: 55555-39-0

Molecular Formula: C₁₅H₂₀O₃

Molecular Weight: 248.321

Accurate Mass: 248.141245

Percentage Composition: C 72.55%; H 8.12%; O 19.33%

Biological Source: Isol. from *Dittrichia* spp., *Inula* spp., *Pulicaria* spp. and *Xanthium* spp.

Physical Description: Oil

Optical Rotation: [α]_D²⁴ -38.9 (c, 0.44 in CHCl₃)