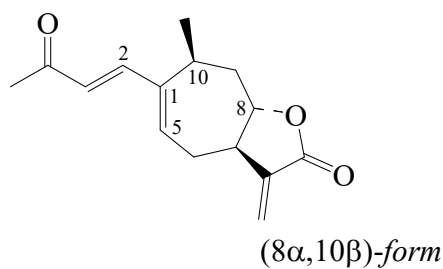




>>Entry Name: 4-Oxo-1(5),2,11(13)-xanthatrien-12,8-olide



**Molecular Formula:** C<sub>15</sub>H<sub>18</sub>O<sub>3</sub>

**Molecular Weight:** 246.305

**Accurate Mass:** 246.125595

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

>>Variant: (8 $\alpha$ ,10 $\beta$ )-form

**Synonym(s):** Xanthatin

**CAS Registry Number:** 26791-73-1

**Molecular Formula:** C<sub>15</sub>H<sub>18</sub>O<sub>3</sub>

**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:** [ $\alpha$ ]<sub>D</sub> -20

**Solubility:** BERDY SOL: Sol. MeOH, Et<sub>2</sub>O; poorly sol. H<sub>2</sub>O, bases, hexane

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

**Hazard & Toxicity:** BERDY HAZD : LD<sub>50</sub> (mus, ipr) 800 mg/kg

>>Derivative: 1 $\alpha$ ,5 $\alpha$ -Epoxide

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

**Molecular Formula:** C<sub>15</sub>H<sub>18</sub>O<sub>4</sub>

**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 $\beta$ ,5 $\beta$ -Epoxide

**Synonym(s):** 1 $\beta$ ,5 $\beta$ -Epoxyxanthatin

**Molecular Formula:** C<sub>15</sub>H<sub>18</sub>O<sub>4</sub>

**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:** C<sub>15</sub>H<sub>20</sub>O<sub>3</sub>

**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:** [ $\alpha$ ]<sub>D</sub><sup>24</sup> -38.9 (c, 0.44 in CHCl<sub>3</sub>)