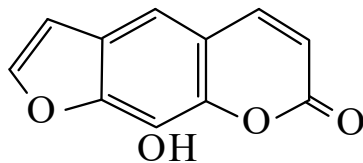




**>>Entry Name: Xanthotoxol**

**Synonym(s):** 9-Hydroxy-7*H*-furo[3,2-*g*][1]benzopyran-7-one, 9C1



**CAS Registry Number:** 2009-24-7

**Molecular Formula:** C<sub>11</sub>H<sub>6</sub>O<sub>4</sub>

**Molecular Weight:** 202.166

**Accurate Mass:** 202.02661

**Percentage Composition:** C 65.35%; H 2.99%; O 31.66%

**Biological Source:** Isol. from *Cnidium dubium*, *Cryptodiscus didymus*, *Evodia hupehensis*, *Selinum tenuifolium*, *Aegle marmelos*, *Angelica archangelica*, *Pastinaca* spp., *Poncirus trifoliata* etc.

**Physical Description:** Cryst. (EtOH aq.)

**Melting Point:** Mp 251-252°

**Hazard & Toxicity:** LD<sub>50</sub> (rat, orl) 480 mg/kg ; BERDY HAZD : LD<sub>50</sub> (rat, orl) 480 mg/kg

**>>Derivative:** *O*-β-L-Arabinopyranoside

**Synonym(s):** Xanthotoxol arabinoside

**CAS Registry Number:** 160845-06-7

**Molecular Formula:** C<sub>16</sub>H<sub>14</sub>O<sub>8</sub>

**Molecular Weight:** 334.282

**Accurate Mass:** 334.06887

**Percentage Composition:** C 57.49%; H 4.22%; O 38.29%

**Biological Source:** Constit. of *Ruta graveolens*

**Physical Description:** Needles

**Melting Point:** Mp 180-182°

**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>25</sup> +12 (MeOH)

**UV:** [neutral]  $\lambda_{\max}$  220 (); 250 (); 260 (); 300 () (no solvent reported)

**>>Derivative:** *O*-β-D-Glucopyranoside

**Molecular Formula:** C<sub>17</sub>H<sub>16</sub>O<sub>9</sub>

**Molecular Weight:** 364.308

**Accurate Mass:** 364.079435

**Percentage Composition:** C 56.05%; H 4.43%; O 39.53%

**Biological Source:** Constit. of *Aegle marmelos*

**Physical Description:** Cryst.

**Melting Point:** Mp 219-220°

**>>Derivative:** Me ether

**>>Derivative:** *O*-(3-Methyl-2-butenyl)

**>>Derivative:** *O*-(3-Methyl-3-butenyl)

**Synonym(s):** Ferulidene

**CAS Registry Number:** 55747-78-9

**Molecular Formula:** C<sub>16</sub>H<sub>14</sub>O<sub>4</sub>

**Molecular Weight:** 270.284

**Accurate Mass:** 270.08921

**Percentage Composition:** C 71.10%; H 5.22%; O 23.68%

**Biological Source:** Constit. of *Prangos ferulacea*

**Physical Description:** Cryst.

**Melting Point:** Mp 119-120°

**>>Derivative:** *O*-(2,3-Epoxy-3-methylbutyl)