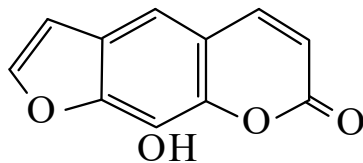




>>Entry Name: Xanthotoxol

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



CAS Registry Number: 2009-24-7

Molecular Formula: C₁₁H₆O₄

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: LD₅₀ (rat, orl) 480 mg/kg ; BERDY HAZD : LD₅₀ (rat, orl) 480 mg/kg

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

Synonym(s): Xanthotoxol arabinoside

CAS Registry Number: 160845-06-7

Molecular Formula: C₁₆H₁₄O₈

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: [α]_D²⁵ +12 (MeOH)

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

>>Derivative: *O*-β-D-Glucopyranoside

Molecular Formula: C₁₇H₁₆O₉

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: C₁₆H₁₄O₄

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)