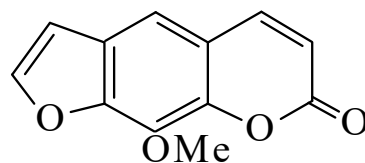




>>Entry Name: Xanthotoxin

Synonym(s): 9-Methoxy-7*H*-furo[3,2-*g*][1]benzopyran-7-one, 9Cl, 8Cl. 9-Methoxyfuro[3,2-*g*]chromen-7-one. 8-Methoxy-4',5':6,7-furocoumarin. 9-Methoxypsoralen. 8-Methoxypsoralen. **Methoxsalen**, BAN. Zanthotoxin. Ammoidin. Meloxine. Methoxa-Dome. Geroxalen. Oxsoralen



CAS Registry Number: 298-81-7

Molecular Formula: C₁₂H₈O₄

Molecular Weight: 216.193

Accurate Mass: 216.04226

Percentage Composition: C 66.67%; H 3.73%; O 29.60%

Biological Source: Isol. from *Cnidium dubium*, *Cryptodiscus didymus*, *Evodia hupehensis*, *Selinum tenuifolium*, *Aegle marmelos* and other plants

Use/Importance: Radioprotectant. Photosensitiser

Biological Use/Importance: Antiinflammatory, spasmolytic agent. Used with UV light in treatment of psoriasis and other skin disorders. Dermatological agent.

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 148°

Solubility: BERDY SOL: Sol. EtOH

Calculated Log P Data: Log P 2.3 (calc)

UV: [neutral] $\lambda_{\max}$ 218 (ϵ 25300); 248 (ϵ 24600); 299 (ϵ 12400) (MeOH) [neutral] $\lambda_{\max}$ 219 (ϵ 30000); 249 (ϵ 28800); 301 (ϵ 14400) (EtOH) (Berdy)

Other Data: Bitter tasting with tingling sensation

Hazard & Toxicity: Human carcinogen (IARC) in combination with UV light. LD₅₀ (rat, orl) 791 mg/kg

Aldrich: 23272-6

Fluka: 95560

Sigma: M3501

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