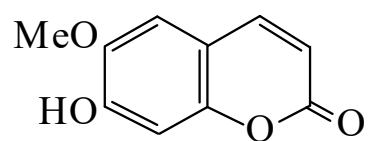




>>Entry Name: 7-Hydroxy-6-methoxy-2*H*-1-benzopyran-2-one, 9CI

ENTRY UNDER REVIEW

Synonym(s): 7-Hydroxy-6-methoxycoumarin. **Scopoletin**. Aesculetin 6-methyl ether. Chrysotropic acid. Gelseminic acid. β -Methylaesculetin. Buxuletin. Escopoletin. Scopoletol. Baogongteng B



CAS Registry Number: 92-61-5

Related CAS Registry Numbers(s): 13544-37-1 73435-97-9

Molecular Formula: C₁₀H₈O₄

Molecular Weight: 192.171

Accurate Mass: 192.04226

Percentage Composition: C 62.50%; H 4.20%; O 33.30%

Biological Source: Occurs widely in the plant world, for example, the root of *Gelsemium sempervirens*, *Atropa belladonna*, *Convolvulus scammonia*, *Ipomoea orizabensis*, *Prunus serotina*, *Fabiana imbricata* and also *Diospyros* spp., *Peucedanum* spp., *Heracleum* spp., *Skimmia* spp. Also occurs in the Chinese crude drug Toki (from *Angelica acutiloba*)

Use/Importance: Antispasmodic agent

Physical Description: Needles or prisms (EtOH)

Melting Point: Mp 204°

Solubility: BERDY SOL: Sol. MeOH, C₆H₆

Calculated Log P Data: Log P 1.33 (calc)

UV: [neutral] $\lambda_{\max}$ 229 (ϵ 13800); 252 (ϵ 9120); 260 (sh) (ϵ 8710); 297 (ϵ 9550); 344 (ϵ 13500) (MeOH) (Derep) [neutral] $\lambda_{\max}$ 230 (); 255 (); 295 (); 345 () (MeOH) (Berdy) [neutral] $\lambda_{\max}$ 228 (ϵ 23000); 254 (ϵ 7600); 297 (ϵ 8700); 345 (ϵ 20500) (EtOH) (Berdy)

Other Data: Reduces Fehling's and Tollen's reagents

Hazard & Toxicity: LD₅₀ (rat, orl) 3800 mg/kg

Aldrich: 24658-1

Fluka: 84792

Sigma: S2500

>>Derivative: Ac

Synonym(s): 7-Acetoxy-6-methoxycoumarin

CAS Registry Number: 56795-51-8

Molecular Formula: C₁₂H₁₀O₅

Molecular Weight: 234.208

Accurate Mass: 234.052825

Percentage Composition: C 61.54%; H 4.30%; O 34.16%

Biological Source: Constit. of *Sterculia urens*

Melting Point: Mp 177°

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

Synonym(s): Scopolin. Murrayin

CAS Registry Number: 531-44-2

Molecular Formula: C₁₆H₁₈O₉

Molecular Weight: 354.313

Accurate Mass: 354.095085

Percentage Composition: C 54.24%; H 5.12%; O 40.64%

Biological Source: Isol. from *Scopolia japonica*, *Hedera helix* and others

Melting Point: Mp 217-219°

UV: [neutral] $\lambda_{\max}$ 227 (ϵ 19200); 340 (ϵ 9800) (MeOH) (Berdy)