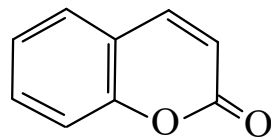




>>Entry Name: **2H-1-Benzopyran-2-one**, 9CI

Synonym(s): Coumarin. Coumarinic anhydride. α -Benzopyrone. Cumarin



CAS Registry Number: 91-64-5

Molecular Formula: C₉H₆O₂

Molecular Weight: 146.145

Accurate Mass: 146.03678

Percentage Composition: C 73.97%; H 4.14%; O 21.90%

Biological Source: Occurs in woodruff (*Coumarouna odorata*) melilot, tonka beans, lavender oil and other plants. Produced by Perkin reaction between 2-Hydroxybenzaldehyde [HHB01-Z](#) and Acetic anhydride [DFR94-Z](#) or by the Raschig method from 2-Methylphenol [DXH33-E](#)

Use/Importance: Antineoplastic, antiinflammatory, antihyperglycaemic agent. Used for treatment of lymphoedema. Used extensively in perfumery

Physical Description: Rhombic cryst.

Melting Point: Mp 70°

Boiling Point: Bp 291°

Solubility: Sol. EtOH, hot H₂O, alkalis; BERDY SOL: Sol. MeOH, Et₂O; poorly sol. H₂O

Calculated Log P Data: Log P 1.41 (calc)

UV: [neutral] $\lambda_{\max}$ 273 (ϵ 10960); 307 (ϵ 5623) (MeOH) (Berdy)

Other Data: Hydrol. by hot conc. alkalis

Hazard & Toxicity: Banned by FDA for use in food. LD₅₀ (rat, orl) 293 kg/kg. Exp. hepatotoxic with species differences between rodent/primate. Exp. teratogen

Aldrich: W50430-0

Fluka: 28150

Sigma: C4261

>>Derivative: Hydrazone

CAS Registry Number: 5841-34-9

Physical Description: Yellow cryst. (MeOH)

Melting Point: Mp 85-86°

>>Derivative: Semicarbazone

Physical Description: Light yellow cryst. (EtOH aq.)

Melting Point: Mp 218-220°

>>Derivative: Di-Et acetal

Synonym(s): 2,2-Diethoxy-2H-1-benzopyran

CAS Registry Number: 33871-81-7

Molecular Formula: C₁₃H₁₆O₃

Molecular Weight: 220.268

Accurate Mass: 220.109945

Percentage Composition: C 70.89%; H 7.32%; O 21.79%

Physical Description: Liq.

Boiling Point: Bp₁₀ 134-136°. Bp_{0.5} 104°

Other Data: Hydrol. to 2H-1-Benzopyran-2-one [HBX68-O](#)

References: