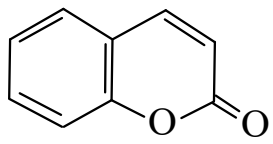
>>**Entry Name: 2*H*-1-Benzopyran-2-one,** 9CI
Synonym(s): Coumarin. Coumarinic anhydride. α-Benzopyrone. Cumarin



CAS Registry Number: 91-64-5

Molecular Formula: $C_9H_6O_2$
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 H_2O, alkalis; BERDY SOL: Sol. MeOH, Et_2O; poorly sol. H_2O
Calculated Log P Data: Log P 1.41 (calc)
UV: [neutral] λ_{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. LD_{50} (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-2*H*-1-benzopyran

CAS Registry Number: 33871-81-7
Molecular Formula: $C_{13}H_{16}O_3$
Molecular Weight: 220.268
Accurate Mass: 220.109945
Percentage Composition: C 70.89%; H 7.32%; O 21.79%
Physical Description: Liq.
Boiling Point: Bp_{10} 134-136°. $Bp_{0.5}$ 104°
Other Data: Hydrol. to 2*H*-1-Benzopyran-2-one HBX68-O

References: