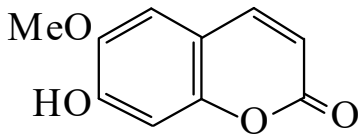
>>**Entry Name: 7-Hydroxy-6-methoxy-2*H*-1-benzopyran-2-one,** 9CI
ENTRY UNDER REVIEW

Synonym(s): 7-Hydroxy-6-methoxycoumarin. **Scopoletin.** Aesculetin 6-methyl ether. Chrysatropic 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: $C_{10}H_8O_4$
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, C_6H_6
Calculated Log P Data: Log P 1.33 (calc)
UV: [neutral] λ_{max} 229 (ε 13800); 252 (ε 9120); 260 (sh) (ε 8710); 297 (ε 9550); 344 (ε 13500) (MeOH) (Derep) [neutral] λ_{max} 230 (); 255 (); 295 (); 345 () (MeOH) (Berdy) [neutral] λ_{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: LD_{50} (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: $C_{12}H_{10}O_5$
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: $C_{16}H_{18}O_9$
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] λ_{max} 227 (ε 19200); 340 (ε 9800) (MeOH) (Berdy)