



Formula: C₁₀H₈O₄

MW: 192.17

CAS: 92-61-5

MDL: MFCD00006872

TNP: TNP00096



LogP: 0.95

LogS:

Acceptors: 4

Donors: 1

Rotation Bonds: 2

Chiral Centers: 0

N+O: 4

LIPINSKY: 4

IUPAC: 7-hydroxy-6-methoxychromen-2-one

Smiles: c12oc(ccc2cc(c(c1)O)OC)=O

Merck 13 Reference: Monograph Number: 0008483

Title: Scopoletin

CAS Registry Number: 92-61-5

CAS Name: 7-Hydroxy-6-methoxy-2H-1-benzopyran-2-one

Additional Names: 7-hydroxy-6-methoxycoumarin; 6-methoxyumbelliferone; b-methylesculetin; chrysotropic acid; gelseminic acid

Molecular Formula: C₁₀H₈O₄

Molecular Weight: 192.17.

Percent Composition: C 62.50%, H 4.20%, O 33.30%

Literature References: The aglucone of scopolin. Occurs in root of *Scopolia japonica* Maxim., *Scopolia carniolica* Jacq., *Atropa belladonna* L., Solanaceae, *Convolvulus scammonia* L., Convolvulaceae. Isoln: Eykman, Ber. 17 III, 442 (1884). Synthesis: Crosby, J. Org. Chem. 26, 1215 (1961); Desai, Desai, J. Indian Chem. Soc. 40, 456 (1963).

Properties: Needles or prisms from chloroform or acetic acid, mp 204. uv max: 230, 254, 260, 298, 346 nm (log e 4.11, 3.68, 3.63, 3.68, 4.07), Ballantyne et al., Tetrahedron 27, 871 (1971). Slightly sol in water or cold alcohol; sol in hot alcohol or hot glacial acetic acid; moderately sol in chloroform. Practically insol in benzene. Its alcoholic soln has a blue fluorescence. Reduces Fehling's soln.

Melting point: mp 204

Absorption maximum: uv max: 230, 254, 260, 298, 346 nm (log e 4.11, 3.68, 3.63, 3.68, 4.07), Ballantyne et al., Tetrahedron 27, 871 (1971)