



Formula: C₁₁H₆O₃

MW: 186.17

CAS: 66-97-7

MDL: MFCD00010520

TNP: TNP00293

PSORALEN; 7H-FURO[3,2-G][1]BENZOPYRAN-7-ONE; 7h-furo[3,2-g]benzopyran-7-one; FURO[3,2-G]BENZOPYRAN-7-ONE; FURO[3,2-G]COUMARIN; FICUSIN; 2-Propenoic acid, 3-(6-hydroxy-5-benzofuranyl)-, delta-lactone; 2-Propenoicacid,3-(6-hydroxy-5-benzofuranyl)-,d-lactone



LogP: 14.41

LogS: -9.06

Acceptors: 3

Donors: 0

Rotation Bonds: 0

Chiral Centers: 0

N+O: 3

LIPINSKY: 3

Info: psoralens are phytoalexins; they are used by plants in a defensive response to attacks by fungi and insects

IUPAC: furano[3,2-g]chromen-2-one

Smiles: O=c1oc2c(cc1)cc1c(c2)occ1

SOURCE: Furocoumarin occurring in more than dozen plant sources.

Specification: Coumarins; Intermediates & Fine Chemicals; Pharmaceuticals Psoralen
Chemical Properties:

mp 160-162 C storage temp. 2-8C Merck 13,8019 CAS DataBase Reference66-97-7(CAS
DataBase Reference) NIST Chemistry Reference7H-furo[3,2-g][1]benzopyran-7-one(66-97-7)
Safety Information Hazard Codes Xn Risk Statements 22-36/37/38 Safety Statements 26 WGK
Germany 3 RTECS LV0944000 F 8-10 Hazardous Substances Data66-97-7(Hazardous
Substances Data) Psoralen Usage And Synthesis Chemical Properties:

Crystalline Solid UsageUse as photochemical probe in biological systems Psoralen

Merck 13 Reference: Monograph Number: 0008019

Title: Psoralen

CAS Registry Number: 66-97-7

CAS Name: 7H-Furo[3,2-g][1]benzopyran-7-one

Additional Names: 6-hydroxy-5-benzofuranacrylic acid d-lactone; furo[3,2-g]coumarin; ficusin

Molecular Formula: C₁₁H₆O₃

Molecular Weight: 186.16.

Percent Composition: C 70.97%, H 3.25%, O 25.78%

Literature References: One of a group of furocoumarins occurring naturally in more than two
dozen plant sources, including Rutaceae (e.g. bergamot, limes, cloves), Umbelliferae (e.g.
celery, parsnips), Leguminosae (e.g. Psoralen coryfolia), and Moraceae (e.g. figs). Isoln: H. S.
Jois et al., J. Indian Chem. Soc. 10, 41 (1933); A. Stoll et al., Helv. Chim. Acta 33, 1637 (1950);
F. E. King et al., J. Chem. Soc. 1954, 1392. Synthesis: E. Sp