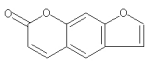

Formula: C11H6O3

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 rsponse 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