



Formula: C<sub>11</sub>H<sub>6</sub>O<sub>3</sub>

MW: 186.17

CAS: 523-50-2

TNP NUMBER: TNP00431

MDL NUMBER: MFCD00064930

IUPAC: furano[2,3-h]chromen-8-one

Smiles: c1cc2ccc(oc2c2c1occ2)=O

Photosensitizing; used for determining DNA/RNA structures in cells and microorganisms.

REFERENCE: Bordin, F., et al., Angelicins, angular analogs of psoralens: chemistry, photochemical, photobiological and phototherapeutic properties. *Pharmacol. Ther.* 52, 331-363, (1991) Ebermann, R., et al., Natural products derived from plants as potential drugs for the photodynamic destruction of tumor cells. *J. Photochem. Photobiol. B, Biol.* 36, 95-97, (1996)

SOURCE: Furocoumarin C<sub>11</sub>H<sub>6</sub>O<sub>3</sub> from plants of the Psoralea genus, Leguminosae.

ACCEPTORS: 3

DONORS: 0

ROTATION BONDS: 0

N+O: 3

Chiral Centers: 0

LogP: 2.56

LogS: -3.58

LIPINSKI: 4

Synonyms:

ANGELICIN;ANGELICINE;ISOBERGAPTEN;ISOPSORALEN;ISOPSORALENE;2-OXO-[2H]-FURO[2,3-H]-1-BENZOPYRAN;2h-furo(2,3-h)(1)benzopyran-2-one;2h-furo(2,3-h)-1-benzopyran-2-one

CAS:523-50-2

MF:C11H6O3

MW:186.16

EINECS:

Product Categories:Coumarins;Miscellaneous Natural Products;Heterocyclic Compounds;Heterocycles 2-Oxo-(2H)-furo(2,3-h)-1-benzopyran

Chemical Properties: mp 132-134C storage temp. 2-8C

CAS DataBase Reference: 523-50-2(

CAS DataBase Reference: ) NIST Chemistry

Reference2H-furo[2,3-h]-1-benzopyran-2-one(523-50-2) Xn,Xi Risk Statements 20/21/22-36/37/38-40 Safety Statements 26-36/37/39-37/39-36 WGK Germany 3 RTECS LV0940000 Hazardous Substances Data523-50-2(Hazardous Substances Data) 2-Oxo-(2H)-furo(2,3-h)-1-benzopyran

Usage And Synthesis:

Chemical Properties: White Solid UsageAntifungal 2-Oxo-(2H)-furo(2,3-h)-1-benzopyran

