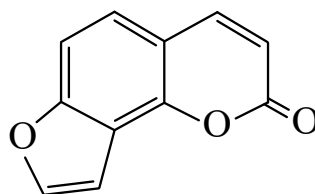




>>Entry Name: **2*H*-Furo[2,3-*h*][1]benzopyran-2-one, 9Cl**

ENTRY UNDER REVIEW

Synonym(s): **Angelicin**‡. Isopsoralen. Furo[5',4':7,8]coumarin. Bakuchicin



CAS Registry Number: 523-50-2

Molecular Formula: C₁₁H₆O₃

Molecular Weight: 186.167

Accurate Mass: 186.031695

Percentage Composition: C 70.97%; H 3.25%; O 25.78%

Biological Source: Constit. of roots and leaves of angelica (*Angelica archangelica*). Found in roots and on surface of parsnips and diseased celery. Also in other *Angelica* spp, *Heracleum* spp. and others

Use/Importance: Possesses sedative props.

Melting Point: Mp 138-139.5°

Calculated Log P Data: Log P 1.97 (calc)

Other Data: Struct. of Bakuchicin revised (1995)

Hazard & Toxicity: Prob. a weak photocarcinogen. LD₅₀ (rat, orl) 322 mg/kg ; BERDY HAZD : LD₅₀ (rat, orl) 322 mg/kg

Sigma: A0956

>>Derivative: 5-Hydroxy

see Isobergaptol, [LLM96-C](#)

>>Derivative: 6-Hydroxy

see 6-Hydroxy-2*H*-furo[2,3-*h*]-1-benzopyran-2-one, [HBV77-G](#)

>>Derivative: 3-Methoxy

Synonym(s): 3-Methoxy-2*H*-furo[2,3-*h*][1]benzopyran-2-one. **3-Methoxyangelicin**

Molecular Formula: C₁₂H₈O₄

Molecular Weight: 216.193

Accurate Mass: 216.04226

Percentage Composition: C 66.67%; H 3.73%; O 29.60%

Biological Source: Constit. of *Pilocarpus riedelianus*

Physical Description: Cryst.

Melting Point: Mp 138-140°

>>Derivative: 3,6-Dimethoxy

Synonym(s): 3,6-Dimethoxy-2*H*-furo[2,3-*h*][1]benzopyran-2-one. **3,6-Dimethoxyangelicin**

Molecular Formula: C₁₃H₁₀O₅

Molecular Weight: 246.219

Accurate Mass: 246.052825

Percentage Composition: C 63.42%; H 4.09%; O 32.49%

Biological Source: Constit. of *Pilocarpus riedelianus*

Physical Description: Amorph. solid

References: