



Formula: C<sub>12</sub>H<sub>8</sub>O<sub>4</sub>

MW: 216.19

CAS: 484-20-8

MDL: MFCD00010272

TNP: TNP00299

2-g)(1)benzopyran-7-one,4-methoxy-7h-furo(; 4-Methoxy-7H-furo(3,2-g)(1)benzopyran-7-one; 4-methoxy-7H-furo[3,2-g][1]benzopyran-7-one; 4-Methoxy-7H-furo[3,2-g]chromen-7-one; 4-Methoxy-furo[3,2-g]chromen-7-one; 5-Methoxy-6,7-furanocoumarin; 6-Hydroxy-4-methoxy-5-



LogP: 4.24

LogS: -4.94

Acceptors: 4

Donors: 0

Rotation Bonds: 1

Chiral Centers: 0

N+O: 4

LIPINSKY: 4

IUPAC: 5-methoxyfurano[3,2-g]chromen-2-one

Smiles: O(C)c1c2c(cc3c1cco3)oc(cc2)=O

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

mp 190-193 C(lit.) storage temp. 2-8C Merck 1157 Stability:Stable. Combustible. Incompatible with strong oxidizing agents. May be light sensitive. CAS DataBase Reference484-20-8(CAS DataBase Reference) NIST Chemistry Reference7H-furo[3,2-g][1]benzopyran-7-one, 4-methoxy-(484-20-8) EPA Substance Registry System7H-Furo[3,2-g][1] benzopyran-7-one, 4-methoxy-(484-20-8) Safety Information Hazard Codes Xi Risk Statements 43 Safety Statements 36/37 WGK Germany 2 RTECS LV1300000 F 8-10 Hazardous Substances Data484-20-8(Hazardous Substances Data) 5-Methoxypsoralen English Bergapten Usage And Synthesis Chemical Properties:

Crystalline Solid UsageNaturally occurring analog of psoralen and isomer of methoxsalen. Found in a wide variety of plants. Antipsoriatic General DescriptionGrayish-white microcrystalline powder or yellow fluffy solid. Air & Water ReactionsInsoluble in water. Reactivity ProfileBergapten may be sensitive to exposure to light. A related chemical is incompatible with strong oxidizers. Fire HazardFlash point data for Bergapten are not available; however, Bergapten is probably combustible. Bergapten Raw materialsSodium hydroxide-->Hydrochloric acid-->Ethyl acetate-->Methanol-->Sulfuric acid -->Dichloromethane-->N,N-Dimethylformamide-->Potassium carbonate-->Chloroform-->Sodium sulfate-->Triethylamine-->Ammonia-->Sodium bicarbonate-->1,4-Dioxane-->Formic acid-->tert-Butanol-->Zinc chloride-->Potassium iodide-->Iodine-->Tetrabutylammonium bromide-->Boron trifluoride etherate-->Palladium diacetate-->2,6-Lutidine-->Allyl bromide-->Sodium periodate-->Osmium tetroxide-->Ethyl propiolate-->Phloroglucinol dihydrate

Merck 13 Reference: Monograph Number: 0001160

Title: Bergapten

CAS Registry Number: 484-20-8

CAS Name: 4-Methoxy-7H-furo[3,2-g][1]benzopyran-7-one

Additional Names: 5-methoxypsoralen; bergapten; bergapten; heraclin; majudin; 5-MOP

Trademarks: Psoraderm-5 (Sunlife)

Molecular Formula: C<sub>12</sub>H<sub>8</sub>O<sub>4</sub>

Molecular Weight: 216.19.

Percent Composition: C 66.67%, H 3.73%, O 29.60%

Literature References: Naturally occurring analog of psoralen and isomer of methoxsalen, q.q.v., found in a wide variety of plants. It was first isolated from oil of bergamot from *Citrus bergamia* Risso, *Aurantiodia*: Pomeranz, *Monatsh. Chem.* 12, 379 (1891), 14, 28 (1893). Isolated from *Fagara xanthoxyloides* Lam., *Rutaceae*: H. Thoms, E. Baetcke, *Ber.* 44, 3326 (1911); 45, 3705 (1912). Synthesis: E. Sp