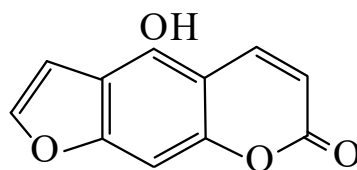




>>Entry Name: Bergaptol

ENTRY UNDER REVIEW

Synonym(s): 4-Hydroxy-7*H*-furo[3,2-*g*][1]benzopyran-7-one, 9Cl. 4-Hydroxypsoralen



CAS Registry Number: 486-60-2

Molecular Formula: C<sub>11</sub>H<sub>6</sub>O<sub>4</sub>

Molecular Weight: 202.166

Accurate Mass: 202.02661

Percentage Composition: C 65.35%; H 2.99%; O 31.66%

Biological Source: Constit. of bergamot oil (*Citrus bergamia*). Also from various other *Citrus* spp.

Physical Description: Needles (EtOAc)

Melting Point: Mp 277-278°

>>Derivative: *O*-β-D-Glucopyranoside

Molecular Formula: C<sub>17</sub>H<sub>16</sub>O<sub>9</sub>

Molecular Weight: 364.308

Accurate Mass: 364.079435

Percentage Composition: C 56.05%; H 4.43%; O 39.53%

Biological Source: Constit. of *Notopterygium forbesii*

Physical Description: Needles (MeOH)

Melting Point: Mp 254-256°

>>Derivative: Me ether

Synonym(s): 4-Methoxy-7*H*-furo[3,2-*g*]benzopyran-7-one. **Bergapten**. Heraclin. Majudin

CAS Registry Number: 484-20-8

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

Molecular Weight: 216.193

Accurate Mass: 216.04226

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

Biological Source: Major constit. of bergamot oil (*Citrus bergamia*), also from *Heracleum giganteum* and *Ammi majus*. Widely distributed in the Rutaceae and Umbelliferae

Use/Importance: Antipsoriatic, antiinflammatory, antihistamine agent. Show spasmolytic props. Used in the treatment of vitiligo

Physical Description: Needles (EtOH)

Melting Point: Mp 188°

Solubility: BERDY SOL: Sol. MeOH, Et<sub>2</sub>O; poorly sol. H<sub>2</sub>O

Calculated Log P Data: Log P 2.3 (calc)

UV: [neutral] λ<sub>max</sub> 222 (ε 22600); 250 (ε 16500); 310 (ε 13600) (MeOH) (Berdy) [neutral] λ<sub>max</sub> 220 (ε 14100); 242 (ε 8000); 268 (ε 10700); 310 (ε 9100) (EtOH) (Berdy)

Other Data: Pastinacin was impure Bergapten

**Hazard & Toxicity:** Skin photosensitiser. Probable human carcinogen. LD<sub>50</sub> (mus, orl) 8100 mg/kg

Aldrich: 27572-7

Fluka: 65320

Sigma: M1648

>>Derivative: *O*-(3-Methyl-2-butenyl)

see Isoimperatorin, [HDN59-C](#)

>>Derivative: *O*-(2,3-Epoxy-3-methylbutyl)

see Oxypeucedanin, [HJP78-H](#)

>>Derivative: *O*-(2,3-Dihydroxy-3-methylbutyl)

see Aviprin, [HBS90-Q](#)

>>Derivative: *O*-(2-Hydroxy-3-methyl-3-butenyl)