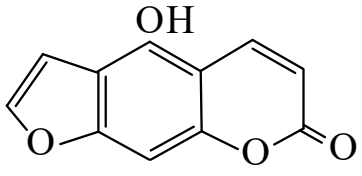
>>**Entry Name: Bergaptol**
ENTRY UNDER REVIEW
Synonym(s): 4-Hydroxy-7*H*-furo[3,2-*g*][1]benzopyran-7-one, 9Cl. 4-Hydroxypsoralen



CAS Registry Number: 486-60-2

Molecular Formula: $C_{11}H_6O_4$
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: $C_{17}H_{16}O_9$
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: $C_{12}H_8O_4$
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_2O; poorly sol. H_2O
Calculated Log P Data: Log P 2.3 (calc)
UV: [neutral] λ_{max} 222 (ε 22600); 250 (ε 16500); 310 (ε 13600) (MeOH) (Berdy) [neutral] λ_{max} 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_{50} (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)