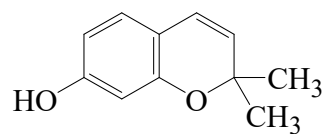




>>Entry Name: **2,2-Dimethyl-2*H*-1-benzopyran-7-ol**, 9CI

Synonym(s): 7-Hydroxy-2,2-dimethyl-2*H*-1-benzopyran. 7-Hydroxy-2,2-dimethylchromene. 2,2-Dimethyl-7-chromenol



CAS Registry Number: 19012-97-6

Molecular Formula: C₁₁H₁₂O₂

Molecular Weight: 176.215

Accurate Mass: 176.08373

Percentage Composition: C 74.98%; H 6.86%; O 18.16%

Physical Description: Yellow oil

Boiling Point: Bp_{0.5} 94-96°

Other Data: Unstable in air

>>Derivative: *O*-β-D-Glucopyranoside

Type of Compound Code(s): VI0030

Molecular Formula: C₁₇H₂₂O₇

Molecular Weight: 338.357

Accurate Mass: 338.136555

Percentage Composition: C 60.35%; H 6.55%; O 33.10%

Biological Source: Constit. of *Ageratum conyzoides*

Physical Description: Oil

Optical Rotation: [α]_D²³ -49.9 (c, 0.2 in EtOH)

>>Derivative: Ac

CAS Registry Number: 19012-98-7

Molecular Formula: C₁₃H₁₄O₃

Molecular Weight: 218.252

Accurate Mass: 218.094295

Percentage Composition: C 71.54%; H 6.47%; O 21.99%

Physical Description: Oil

>>Derivative: 4-Methylbenzenesulfonyl

CAS Registry Number: 100942-31-2

Molecular Formula: C₁₈H₁₈O₄S

Molecular Weight: 330.404

Accurate Mass: 330.09258

Percentage Composition: C 65.43%; H 5.49%; O 19.37%; S 9.71%

Physical Description: Light pink cryst. (MeOH aq.)

Melting Point: Mp 102°

>>Derivative: Me ether

Synonym(s): 7-Methoxy-2,2-dimethyl-2*H*-1-benzopyran, 9CI. 7-Methoxy-2,2-dimethylchromene. Precocene I

CAS Registry Number: 17598-02-6

Type of Compound Code(s): VI0030

Molecular Formula: C₁₂H₁₄O₂

Molecular Weight: 190.241

Accurate Mass: 190.09938

Percentage Composition: C 75.76%; H 7.42%; O 16.82%

Biological Source: From *Ageratum houstonianum* and *Ageratum conyzoides* and from *Verbesina* spp.

Use/Importance: Antiallotropin (induces premature ecdysis in insects)

Physical Description: Liq.

Boiling Point: Bp₁₅ 132-136°

Refractive Index: n_D²⁵ 1.5578

Aldrich: 19585-5

Sigma: M7637

References: