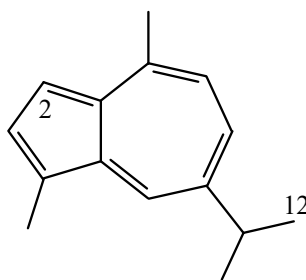




>>Entry Name: 7-Isopropyl-1,4-dimethylazulene

Synonym(s): 1,4-Dimethyl-7-(1-methylethyl)azulene, 9Cl. 1,3,5,7,9-Guaiapentaene. **Guaiazulene**. S-Guaiazulene. Kessazulene. Azulon. Eucazulene. Azunol



CAS Registry Number: 489-84-9

Molecular Formula: C<sub>15</sub>H<sub>18</sub>

Molecular Weight: 198.307

Accurate Mass: 198.14085

Percentage Composition: C 90.85%; H 9.15%

Biological Source: Obt. from essential oils, e.g. chamomile oil. Found also in marine red algae and the gorgonian *Euplexaura erecta*

Use/Importance: Antioxidant, inhibits lipid peroxidation. Antiinflammatory agent, also used to treat gastrointestinal disorders. Hepatoprotectant

Physical Description: Blue-violet plates (EtOH) or blue oil

Melting Point: Mp 31.5°

Boiling Point: Bp<sub>12</sub> 167-168°

Calculated Log P Data: Log P 5.74 (calc)

UV: [neutral] λ<sub>max</sub> 286 (); 292 (); 350 (); 377 (); 600 () (CHCl<sub>3</sub>) (Berdy)

Other Data: λ<sub>max</sub> 556, 581, 603, 632 and 662 nm (Et<sub>2</sub>O)

**Hazard & Toxicity:** LD<sub>50</sub> (rat, orl) 1550 mg/kg

Aldrich: G1100-4

Fluka: 50890

Sigma: G3391

>>Derivative: 1,3,5-Trinitrobenzene complex

CAS Registry Number: 4968-29-0

Physical Description: Black needles (EtOH)

Melting Point: Mp 151-151.5°

>>Derivative: Picrate

Physical Description: Black needles (EtOH)

Melting Point: Mp 122-122.5°

>>Derivative: 2-Bromo

Synonym(s): 2-Bromo-1,3,5,7,9-guaiapentaene. 3-Bromo-7-isopropyl-1,4-dimethylazulene. **3-Bromoguaiazulene**

CAS Registry Number: 90052-61-2

Molecular Formula: C<sub>15</sub>H<sub>17</sub>Br

Molecular Weight: 277.203

Accurate Mass: 276.071361

Percentage Composition: C 64.99%; H 6.18%; Br 28.83%

Biological Source: Constit. of a gorgonian of the Paramuriceidae family

Physical Description: Oil

>>Derivative: 2-Chloro

Synonym(s): 2-Chloro-1,3,5,7,9-guaiapentaene. 3-Chloro-7-isopropyl-1,4-dimethylazulene. **3-Chloroguaiazulene**

CAS Registry Number: 90052-60-1

Molecular Formula: C<sub>15</sub>H<sub>17</sub>Cl

Molecular Weight: 232.752

Accurate Mass: 232.101877

Percentage Composition: C 77.41%; H 7.36%; Cl 15.23%

Biological Source: Constit. of a gorgonian of the Paramuriceidae family

UV: [neutral] λ<sub>max</sub> 246 (ε); 293 (ε); 307 (ε); 352 (ε); 369 (ε); 620 (ε) (CHCl<sub>3</sub>) (Derep)