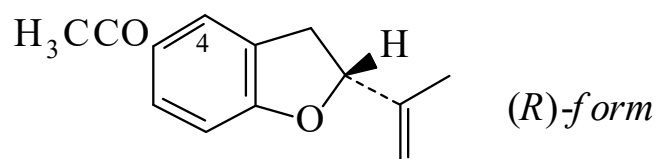




>>Entry Name: Tremetone

Synonym(s): 1-[2,3-Dihydro-2-(1-methylethenyl)-5-benzofuranyl]ethanone, 9Cl. 5-Acetyl-2,3-dihydro-2-isopropenylbenzofuran



Molecular Formula: C<sub>13</sub>H<sub>14</sub>O<sub>2</sub>

Molecular Weight: 202.252

Accurate Mass: 202.09938

Percentage Composition: C 77.20%; H 6.98%; O 15.82%

>>Variant: (R)-form

CAS Registry Number: 4976-25-4

Molecular Formula: C<sub>13</sub>H<sub>14</sub>O<sub>2</sub>

Molecular Weight: 202.252

Accurate Mass: 202.09938

Percentage Composition: C 77.20%; H 6.98%; O 15.82%

Biological Source: Toxic principle in White Snakeroot (*Eupetorium orticaefolium*). Found also in *Baccharis conferta*, *Ageratina altissima*, *Critonia daleoides*, *Parastrephia lepidophylla* and *Podochaenium eminens*

Physical Description: Oil

Optical Rotation:  $[\alpha]_{\text{D}}^{28} -59.6$  (c, 5.5 in EtOH)

UV: [neutral]  $\lambda_{\text{max}}$  207 ( $\epsilon$  5010); 227 ( $\epsilon$  6310); 279 ( $\epsilon$  7940) (MeOH) (Berdy)

>>Derivative: Semicarbazone

Melting Point: Mp 222°

Optical Rotation:  $[\alpha]_{\text{D}}^{28} -56.2$  (c, 0.74 in CHCl<sub>3</sub>)

>>Variant: (±)-form

CAS Registry Number: 35817-04-0

Molecular Formula: C<sub>13</sub>H<sub>14</sub>O<sub>2</sub>

Molecular Weight: 202.252

Accurate Mass: 202.09938

Percentage Composition: C 77.20%; H 6.98%; O 15.82%

Boiling Point: Bp<sub>2</sub> 120-127°

>>Variant: (ξ)-form

Molecular Formula: C<sub>13</sub>H<sub>14</sub>O<sub>2</sub>

Molecular Weight: 202.252

Accurate Mass: 202.09938

Percentage Composition: C 77.20%; H 6.98%; O 15.82%

>>Derivative: 4-Hydroxy

Molecular Formula: C<sub>13</sub>H<sub>14</sub>O<sub>3</sub>

Molecular Weight: 218.252

Accurate Mass: 218.094295

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

Biological Source: Constit. of *Lasiolaena morii*

Physical Description: Gum

References:

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Kawase, Y. *et al.*, *Chem. Lett.*, 1978, 253, (*synth*)

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Bohlmann, F. *et al.*, *Phytochemistry*, 1982, **21**, 161, (*deriv*)

Banskota, A.H. *et al.*, *J. Nat. Prod.*, 1998, **61**, 896-900, (*isol, uv, ir, pmr, cmr, ms*)