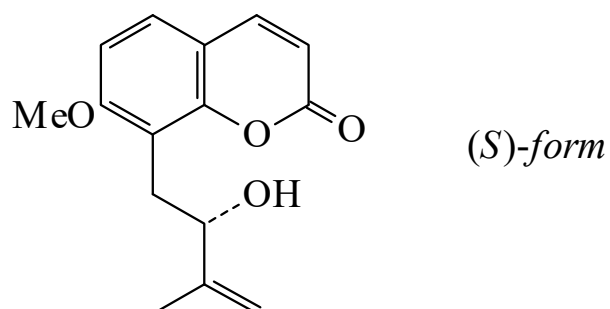




>>Entry Name: Auraptenol

ENTRY UNDER REVIEW

Synonym(s): 8-(2-Hydroxy-3-methyl-3-butenyl)-7-methoxy-2*H*-1-benzopyran-2-one, 9Cl. 8-(2-Hydroxy-3-methyl-3-butenyl)-7-methoxycoumarin



Molecular Formula: C₁₅H₁₆O₄

Molecular Weight: 260.289

Accurate Mass: 260.10486

Percentage Composition: C 69.22%; H 6.20%; O 24.59%

>>Variant: (*S*)-form

CAS Registry Number: 1221-43-8

Molecular Formula: C₁₅H₁₆O₄

Molecular Weight: 260.289

Accurate Mass: 260.10486

Percentage Composition: C 69.22%; H 6.20%; O 24.59%

Biological Source: Constit. of Seville bitter orange (*Citrus aurantium*, sub. sp. *amara*) oil

Physical Description: Needles (EtOH)

Melting Point: Mp 109-110°

Optical Rotation: $[\alpha]_D^{26} +14$ (c, 1 in EtOH)

>>Derivative: 2'-Deoxy, 2'-hydroperoxy

Synonym(s): Peroxyauraptenol

CAS Registry Number: 109741-39-1

Molecular Formula: C₁₅H₁₆O₅

Molecular Weight: 276.288

Accurate Mass: 276.099775

Percentage Composition: C 65.21%; H 5.84%; O 28.95%

Biological Source: Constit. of *Murraya exotica*

Physical Description: Prisms

Melting Point: Mp 114-116°

Optical Rotation: $[\alpha]_D +3.53$ (CHCl₃)

>>Derivative: 2'-Ketone

Synonym(s): 7-Methoxy-8-(3-methyl-2-oxo-3-butenyl)-2*H*-1-benzopyran-2-one, 9Cl. **Murrayone**, Prangone

CAS Registry Number: 19668-69-0

Molecular Formula: C₁₅H₁₄O₄

Molecular Weight: 258.273

Accurate Mass: 258.08921

Percentage Composition: C 69.76%; H 5.46%; O 24.78%

Biological Source: Constit. of *Murraya exotica* and *Prangos ferulacea*

Melting Point: Mp 130°

>>Variant: (±)-form

CAS Registry Number: 61235-25-4

Molecular Formula: C₁₅H₁₆O₄

Molecular Weight: 260.289

Accurate Mass: 260.10486

Percentage Composition: C 69.22%; H 6.20%; O 24.59%

Physical Description: Cryst. (C₆H₆/hexane)

Melting Point: Mp 109-110°

References: