



>>Variant: (S)-form

Synonym(s): Decursinol

CAS Registry Number: 23458-02-8

Molecular Formula: C₁₄H₁₄O₄

Molecular Weight: 246.262

Accurate Mass: 246.08921

Percentage Composition: C 68.28%; H 5.73%; O 25.99%

Biological Source: From roots of *Angelica gigas*

Physical Description: Cryst. (EtOH)

Melting Point: Mp 177°

Optical Rotation: $[\alpha]_D^{17} +104.2$ (c, 0.7 in EtOH)

>>Derivative: Ac

Melting Point: Mp 138-139°

Optical Rotation: $[\alpha]_D^{17} +45.7$

>>Derivative: O-(3-Methyl-2-butenoyl)

Synonym(s): Decursin

CAS Registry Number: 5928-25-6

Molecular Formula: C₁₉H₂₀O₅

Molecular Weight: 328.364

Accurate Mass: 328.131075

Percentage Composition: C 69.50%; H 6.14%; O 24.36%

Biological Source: Isol. from root of *Angelica decursiva*

Physical Description: Prisms (EtOH)

Melting Point: Mp 110-111°

Optical Rotation: $[\alpha]_D^{15} +172.9$ (CHCl₃)

UV: [neutral] $\lambda_{\max}$ 220 () (MeOH) (Berdy)

>>Derivative: 2-Methyl-2-butenoyl(Z-)

Synonym(s): Acutilobin. Decursinol angelate

CAS Registry Number: 130848-06-5

Molecular Formula: C₁₉H₂₀O₅

Molecular Weight: 328.364

Accurate Mass: 328.131075

Percentage Composition: C 69.50%; H 6.14%; O 24.36%

Biological Source: Constit. of *Angelica acutiloba* and *Angelica gigas*

Use/Importance: Antitumour agent

Physical Description: Prisms (MeOH)

Melting Point: Mp 94-95°

Optical Rotation: $[\alpha]_D^{15} +172.9$ (c, 1.3 in CHCl₃)

>>Variant: (±)-form

CAS Registry Number: 15575-65-2

Molecular Formula: C₁₄H₁₄O₄

Molecular Weight: 246.262

Accurate Mass: 246.08921

Percentage Composition: C 68.28%; H 5.73%; O 25.99%

Physical Description: Needles (petrol/EtOAc)

Melting Point: Mp 167.5-168.5°

References: