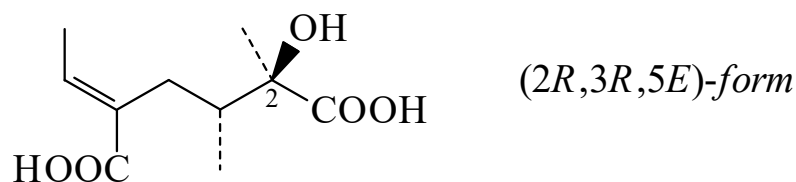




>>Entry Name: 5-Ethylidene-2-hydroxy-2,3-dimethylhexanedioic acid, 9CI

Synonym(s): 6-Hydroxy-5-methyl-2-heptene-3,6-dicarboxylic acid



CAS Registry Number: 6703-97-5

Related CAS Registry Numbers(s): 10407-75-7

Molecular Formula: C₁₀H₁₆O₅

Molecular Weight: 216.233

Accurate Mass: 216.099775

Percentage Composition: C 55.55%; H 7.46%; O 37.00%

>>Variant: (2R,3R,5E)-form

Synonym(s): Integerrinecic acid

CAS Registry Number: 469-45-4

Molecular Formula: C₁₀H₁₆O₅

Molecular Weight: 216.233

Accurate Mass: 216.099775

Percentage Composition: C 55.55%; H 7.46%; O 37.00%

Biological Source: Necic acid from pyrrolizidine alkaloids

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 149-150°

Optical Rotation: $[\alpha]_D^{18} +15.9$ (c, 1 in EtOH)

>>Derivative: Bis-4-phenylphenacyl ester

Melting Point: Mp 100-101°

>>Derivative: δ -Lactone

CAS Registry Number: 34081-94-2

Molecular Formula: C₁₀H₁₄O₄

Molecular Weight: 198.218

Accurate Mass: 198.08921

Percentage Composition: C 60.59%; H 7.12%; O 32.29%

Melting Point: Mp 153°

Optical Rotation: $[\alpha]_D^{25} +40$ (c, 0.94 in EtOH)

>>Variant: (2R,3R,5Z)-form

Synonym(s): Senecic acid. Senecionic acid

CAS Registry Number: 13588-16-4

Molecular Formula: C₁₀H₁₆O₅

Molecular Weight: 216.233

Accurate Mass: 216.099775

Percentage Composition: C 55.55%; H 7.46%; O 37.00%

Biological Source: Necic acid component of pyrrolizidine alkaloids, e.g. Senecionine

Melting Point: Mp 151°

Optical Rotation: $[\alpha]_D +11.8$ (c, 2 in EtOH)

>>Derivative: Bis-4-phenylphenacyl ester

Physical Description: Amorph. (EtOH)

Melting Point: Mp 100-101°

>>Derivative: δ -Lactone

CAS Registry Number: 28822-16-4

Melting Point: Mp 129-130°

Other Data: (E)-lactone is formed if lactonisation is carried out under normal conditions