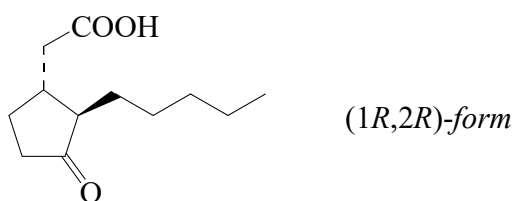




>>Entry Name: 3-Oxo-2-pentylcyclopentaneacetic acid, 9CI



CAS Registry Number: 3572-64-3

Molecular Formula: C₁₂H₂₀O₃

Molecular Weight: 212.288

Accurate Mass: 212.141245

Percentage Composition: C 67.89%; H 9.50%; O 22.61%

>>Variant: (1R,2R)-form

Synonym(s): Dihydrojasmonic acid

CAS Registry Number: 98674-52-3

Molecular Formula: C₁₂H₂₀O₃

Molecular Weight: 212.288

Accurate Mass: 212.141245

Percentage Composition: C 67.89%; H 9.50%; O 22.61%

Biological Source: Isol. from *Vicia faba* and *Secale cereale*

Physical Description: Oil

Optical Rotation: $[\alpha]_D^{22}$ -28.3 (c, 0.1 in MeOH)

>>Derivative: Me ester

Synonym(s): Methyl dihydrojasmonate. Hedione. FEMA 3408

CAS Registry Number: 24851-98-7

Molecular Formula: C₁₃H₂₂O₃

Molecular Weight: 226.315

Accurate Mass: 226.156895

Percentage Composition: C 68.99%; H 9.80%; O 21.21%

Biological Source: Odiferous component in jasmine oil (*Jasminum grandiflorum*)

Use/Importance: Important perfumery ingredient, also used in flavourings

Physical Description: Liq.

Boiling Point: Bp₃ 102-108° (Bp₄ 118-119°)

>>Variant: (1R,2S)-form

Synonym(s): Dihydroisojasmonic acid

CAS Registry Number: 96844-45-0

Molecular Formula: C₁₂H₂₀O₃

Molecular Weight: 212.288

Accurate Mass: 212.141245

Percentage Composition: C 67.89%; H 9.50%; O 22.61%

Biological Source: Isol. from *Botryodiplodia theobromae*

Optical Rotation: $[\alpha]_D^{25}$ +10.5 (c, 0.1 in MeOH)

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