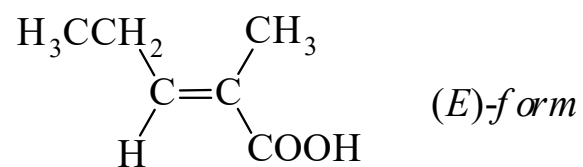




>>Entry Name: 2-Methyl-2-pentenoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): 3-Ethyl-2-methylacrylic acid. 2-Pentene-2-carboxylic acid. FEMA 3195



CAS Registry Number: 3142-72-1

Related CAS Registry Numbers(s): 89301-90-6 134176-70-8 134732-07-3

Molecular Formula: C₆H₁₀O₂

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Use/Importance: Flavouring ingredient

>>Variant: (E)-form

CAS Registry Number: 16957-70-3

Molecular Formula: C₆H₁₀O₂

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Melting Point: Mp 24.1°

Boiling Point: Bp₁₀ 106.5°

Aldrich: 26477-6

>>Derivative: Me ester

CAS Registry Number: 1567-14-2

Molecular Formula: C₇H₁₂O₂

Molecular Weight: 128.171

Accurate Mass: 128.08373

Percentage Composition: C 65.60%; H 9.44%; O 24.97%

Boiling Point: Bp₁₅ 46-47°

Density: d 0.92

Refractive Index: n_D²⁰ 1.4380

>>Derivative: (S)-1-Methylbutyl ester

Synonym(s): Dominicalure 1

CAS Registry Number: 80510-15-2

Molecular Formula: C₁₁H₂₀O₂

Molecular Weight: 184.278

Accurate Mass: 184.14633

Percentage Composition: C 71.70%; H 10.94%; O 17.36%

dominica

Physical Description: Liq.

Optical Rotation: [α]_D +14.2 (c, 1.265 in Et₂O) (= 98% op)

>>Variant: (Z)-form

CAS Registry Number: 1617-37-4

Molecular Formula: C₆H₁₀O₂

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Boiling Point: Bp₁₀ 94-94.4°

>>Derivative: Me ester