



>>Entry Name: 2-Hexenoic acid, 9CI

ENTRY UNDER REVIEW

CAS Registry Number: 1191-04-4

H3CCH2CH2CH=CHCOOH

Molecular Formula: C6H10O2

Molecular Weight: 114.144

Accurate Mass: 114.06808

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

>>Variant: (*E*)-form

Synonym(s): FEMA 3169

CAS Registry Number: 13419-69-7

Molecular Formula: C6H10O2

Molecular Weight: 114.144

Accurate Mass: 114.06808

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

Biological Source: Constit. of root of *Arctium lappa*

Use/Importance: Used as flavouring for tea and reverted soybean oil. Used in hand lotions, etc.

Physical Description: Needles (H2O, EtOH)

Melting Point: Mp 36-37°

Boiling Point: Bp 216-217°. Bp₈ 100°

pKa Value: pK_{a1} 4.75 (25°)

Aldrich: 19308-9

Fluka: 53074

>>Derivative: Me ester

Synonym(s): FEMA 2709

CAS Registry Number: 2396-77-2

Molecular Formula: C7H12O2

Molecular Weight: 128.171

Accurate Mass: 128.08373

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

Biological Source: Present in *Carica* spp., peas and soursop (*Annona muricata*)

Use/Importance: Flavouring ingredient

Physical Description: Liq. with green-fruity flavour

Boiling Point: Bp 169°. Bp₁₃ 56-58°

>>Derivative: 4-Bromophenacyl ester

Melting Point: Mp 62-62.5°

>>Derivative: Chloride

CAS Registry Number: 18802-95-4

Molecular Formula: C6H9ClO

Molecular Weight: 132.589

Accurate Mass: 132.034192

Percentage Composition: C 54.35%; H 6.84%; Cl 26.74%; O 12.07%

Boiling Point: Bp₂₃ 70°

>>Derivative: Anilide

Molecular Formula: C12H15NO

Molecular Weight: 189.257

Accurate Mass: 189.115364

Percentage Composition: C 76.16%; H 7.99%; N 7.40%; O 8.45%

Physical Description: Needles

Melting Point: Mp 109-110°