



>>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°