



**Molecular Weight:** 172.267  
**Accurate Mass:** 172.14633  
**Percentage Composition:** C 69.72%; H 11.70%; O 18.58%  
**Boiling Point:** Bp<sub>18</sub> 77-79°

>>Derivative: 3-Methylbutyl ester

**Synonym(s):** 3-Methylbutyl hexanoate. Isopentyl caproate. FEMA 2075

**CAS Registry Number:** 2198-61-0

**Molecular Formula:** C<sub>11</sub>H<sub>22</sub>O<sub>2</sub>

**Molecular Weight:** 186.294

**Accurate Mass:** 186.16198

**Percentage Composition:** C 70.92%; H 11.90%; O 17.18%

**Use/Importance:** Used in fruit flavours and in fragrance. Present in fruits and alcoholic beverages

**Boiling Point:** Bp 222°

**Density:** d 0.86

>>Derivative: Hexyl ester

**Synonym(s):** Hexyl hexanoate. Capryl caproate. Hexyl caproate. FEMA 2568

**CAS Registry Number:** 6378-65-0

**Molecular Formula:** C<sub>12</sub>H<sub>24</sub>O<sub>2</sub>

**Molecular Weight:** 200.32

**Accurate Mass:** 200.17763

**Percentage Composition:** C 71.95%; H 12.08%; O 15.97%

**Biological Source:** Volatile component from fruit ripening

**Use/Importance:** Used in fruit flavouring

**Physical Description:** Liq.

**Boiling Point:** Bp 245° (208°). Bp<sub>13</sub> 116-120°

**Density:** d<sub>20</sub><sup>20</sup> 0.86

**Refractive Index:** n<sub>D</sub><sup>20</sup> 1.4249

>>Derivative: (E)-2-Hexenyl ester

**Synonym(s):** 2-Hexenyl hexanoate. 2-Hexenyl caproate

**CAS Registry Number:** 53398-86-0

**Molecular Formula:** C<sub>12</sub>H<sub>22</sub>O<sub>2</sub>

**Molecular Weight:** 198.305

**Accurate Mass:** 198.16198

**Percentage Composition:** C 72.68%; H 11.18%; O 16.14%

**Biological Source:** Alarm pheromone of *Riptortus clavatus*

**Boiling Point:** Bp<sub>3</sub> 79°

>>Derivative: Chloride

**CAS Registry Number:** 142-61-0

**Molecular Formula:** C<sub>6</sub>H<sub>11</sub>ClO

**Molecular Weight:** 134.605

**Accurate Mass:** 134.049842

**Percentage Composition:** C 53.54%; H 8.24%; Cl 26.34%; O 11.89%

**Boiling Point:** Bp 151-153°

**Aldrich:** 29465-9

**Fluka:** 21590

**Sigma:** C1899

>>Derivative: Bromide

**CAS Registry Number:** 51499-41-3

**Molecular Formula:** C<sub>6</sub>H<sub>11</sub>BrO

**Molecular Weight:** 179.056

**Accurate Mass:** 178.019326

**Percentage Composition:** C 40.25%; H 6.19%; Br 44.63%; O 8.94%

**Boiling Point:** Bp 175-176°