



>>Entry Name: 3-Hexenoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): 2-Pentene-1-carboxylic acid. Hydrosorbic acid. FEMA 3170

CAS Registry Number: 4219-24-3

Related CAS Registry Numbers(s): 1775-43-5

$\text{H}_3\text{CCH}_2\text{CH}=\text{CHCH}_2\text{COOH}$

Molecular Formula:  $\text{C}_6\text{H}_{10}\text{O}_2$

Molecular Weight: 114.144

Accurate Mass: 114.06808

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

Biological Source: Isol. from raspberry (*Rubus idaeus*) and tea (*Thea sinensis*)

Use/Importance: Used in tea flavouring

Melting Point: Mp 12°

Boiling Point: Bp 208°. Bp<sub>22</sub> 118-119°

Aldrich: W31700-4

>>Variant: (*E*)-form

CAS Registry Number: 1577-18-0

Molecular Formula:  $\text{C}_6\text{H}_{10}\text{O}_2$

Molecular Weight: 114.144

Accurate Mass: 114.06808

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

Aldrich: 19309-7

>>Derivative: Me ester

CAS Registry Number: 2396-78-3

Molecular Formula:  $\text{C}_7\text{H}_{12}\text{O}_2$

Molecular Weight: 128.171

Accurate Mass: 128.08373

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

Biological Source: Constit. of *Asteriscus graveolens*, minor constit. of pineapples

Boiling Point: Bp<sub>34</sub> 67-68°

Other Data: (*E*)-config. assumed

>>Derivative: Et ester

Synonym(s): FEMA 3342

CAS Registry Number: 2396-83-0

Molecular Formula:  $\text{C}_8\text{H}_{14}\text{O}_2$

Molecular Weight: 142.197

Accurate Mass: 142.09938

Percentage Composition: C 67.57%; H 9.92%; O 22.50%

Biological Source: Present in various fruits

Use/Importance: Flavouring agent

Physical Description: Liq. with green, fruity aroma

Boiling Point: Bp<sub>12</sub> 63-64°

Refractive Index: n<sub>D</sub><sup>20</sup> 1.4260

Aldrich: 34029-4

>>Derivative: 2-Propenyl ester

CAS Registry Number: 167773-28-6

Molecular Formula:  $\text{C}_9\text{H}_{14}\text{O}_2$

Molecular Weight: 154.208

Accurate Mass: 154.09938

Percentage Composition: C 70.10%; H 9.15%; O 20.75%

Biological Source: Constit. of the rhizomes of *Ligusticum chuanxiong*

Other Data: (*E*)-config. assumed