>>**Entry Name: Hexanoic acid,** 9CI, 8CI
ENTRY UNDER REVIEW
Synonym(s): Caproic acid. Pentane-1-carboxylic acid. Hexylic acid. Hexoic acid. FEMA 2559

CAS Registry Number: 142-62-1
Related CAS Registry Numbers(s): 10051-44-2

$H_3C(CH_2)_4COOH$

Molecular Formula: $C_6H_{12}O_2$
Molecular Weight: 116.16
Accurate Mass: 116.08373
Percentage Composition: C 62.04%; H 10.41%; O 27.55%
Biological Source: Occurs naturally, e.g. in lichens. Sex pheromone of the female dermestid beetle *Trogoderma glabrum*
Use/Importance: Simple esters are used as flavouring agents. Used for extraction of Co, Mn, Ni and rare earth elements
Physical Description: Oily liq. with acrid taste and unpleasant odour
Melting Point: Fp –1.5°
Boiling Point: Bp 205°
Solubility: Sol. alkalis, EtOH, Et_2O; spar. sol. H_2O
Density: d_4^{15}0.93
pKa Value: pK_{a1} 4.8 (25°)
Refractive Index: n_D^{20} 1.4164
Hazard & Toxicity: Skin and eye irritant. LD_{50} (rat, orl) 3000 mg/kg. Fl. p. 102° (oc), autoignition temp. 380/402°

Aldrich: 15374-5
Fluka: 21530
Sigma: C2250
Supelco: 47-2559

>>**Derivative:** *S*-Benzylthiouronium salt

Melting Point: Mp 146-147°

>>**Derivative:** Me ester
Synonym(s): Methyl hexanoate. Methyl caproate. FEMA 2708

CAS Registry Number: 106-70-7

Molecular Formula: $C_7H_{14}O_2$
Molecular Weight: 130.186
Accurate Mass: 130.09938
Percentage Composition: C 64.58%; H 10.84%; O 24.58%
Biological Source: Present in fruits
Physical Description: Liq. with ether-like odour reminiscent of pineapple
Melting Point: Fp –71°
Boiling Point: Bp 150°. Bp_{15} 52°
Density: d_4^{24}0.885
Refractive Index: n_D^{20} 1.4049
Hazard & Toxicity: Causes burns, flammable, fl. p. 32°

Aldrich: W27081-4
Fluka: 21600
Sigma: C5049

>>**Derivative:** Et ester
Synonym(s): Ethyl hexanoate. Ethyl caproate

CAS Registry Number: 123-66-0

Molecular Formula: $C_8H_{16}O_2$
Molecular Weight: 144.213
Accurate Mass: 144.11503
Percentage Composition: C 66.63%; H 11.18%; O 22.19%
Source/Synthesis: Found in many fruits, Camembert, cheese, milk, fruit brandies, sparkling wine and Bourbon vanilla
Use/Importance: Used in perfumes and fruit flavours
Physical Description: Liq. with strong pineapple odour
Melting Point: Mp –67.5°
Boiling Point: Bp 168°. Bp_2 27°
Density: d