



>>Entry Name: Octadecanoic acid, 9CI

Synonym(s): Stearic acid. Bassinic acid. Lactaric acid. Stearophanic acid. Talgic acid. FEMA 3035. E 570

CAS Registry Number: 57-11-4

Related CAS Registry Numbers(s): 593-29-3 4568-28-9

$\text{H}_3\text{C}(\text{CH}_2)_{16}\text{COOH}$

Molecular Formula: $\text{C}_{18}\text{H}_{36}\text{O}_2$

Molecular Weight: 284.481

Accurate Mass: 284.27153

Percentage Composition: C 76.00%; H 12.75%; O 11.25%

Biological Source: Constit. of most vegetable and animal fats. Manuf. by hydrolysis of fats and oils

Use/Importance: Acid and derivatives widely used as additives to industrial preparations. Used as EtOH soln. for nephelometric detn. of Ca. Used (with heptadecanoic acid) for amino acid sequencing in peptides. Used for surfactants, soaps and plasticisers

Biological Use/Importance: Pharmaceutical excipient (tablet lubricant; Ca and Mg salts are used similarly)

Physical Description: Leaflets

Melting Point: Mp 69.7°

Boiling Point: Bp 386°. Bp₅ 213°

Solubility: Sol. EtOH, C_6H_6 , CHCl_3 ; sl. sol. H_2O

Other Data: Polymorphic, at least 4 cryst. forms are known

Hazard & Toxicity: Skin irritant. Fl. p. 196°, autoignition temp. 395°

Aldrich: 17536-6

Fluka: 85683

Sigma: S4876

>>Derivative: Me ester

Synonym(s): Methyl octadecanoate. Methyl stearate

CAS Registry Number: 112-61-8

Molecular Formula: $\text{C}_{19}\text{H}_{38}\text{O}_2$

Molecular Weight: 298.508

Accurate Mass: 298.28718

Percentage Composition: C 76.45%; H 12.83%; O 10.72%

Melting Point: Mp 39.1°

Boiling Point: Bp₁₅ 215°

Hazard & Toxicity: Fl. p. 153°

Aldrich: 33518-5

Fluka: 85770

Sigma: S8019

>>Derivative: Et ester

Synonym(s): Ethyl octadecanoate. Ethyl stearate

CAS Registry Number: 111-61-5

Molecular Formula: $\text{C}_{20}\text{H}_{40}\text{O}_2$

Molecular Weight: 312.535

Accurate Mass: 312.30283

Percentage Composition: C 76.86%; H 12.90%; O 10.24%

Physical Description: Cryst.

Melting Point: Mp 33.4°. Mp 30.9°

Boiling Point: Bp₁₀ 199°

Hazard & Toxicity: Skin irritant

Aldrich: W34900-3

Fluka: 85690

Sigma: S5251

>>Derivative: Propyl ester

Synonym(s): Propyl octadecanoate. Propyl stearate