



>>Entry Name: Heptadecanoic acid

Synonym(s): Margaric acid. Daturinic acid

CAS Registry Number: 506-12-7

$\text{H}_3\text{C}(\text{CH}_2)_{15}\text{COOH}$

Molecular Formula: $\text{C}_{17}\text{H}_{34}\text{O}_2$

Molecular Weight: 270.454

Accurate Mass: 270.25588

Percentage Composition: C 75.50%; H 12.67%; O 11.83%

Biological Source: Constit. of *Erythrina crista-galli* trunkwood and bark. Common constit. of lipids

Use/Importance: Used (with Stigmast-5-ene-3,7,20-triol [BZJ62-O](#)) for amino acid sequencing in peptides

Physical Description: Cryst. (petrol)

Melting Point: Mp 62-63°

Hazard & Toxicity: LD₅₀ (mus, ivn) 36 mg/kg

Aldrich: H100-0

Fluka: 51610

Sigma: H3500

Supelco: R42-0170

>>Derivative: Me ester

CAS Registry Number: 1731-92-6

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%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 30°

Boiling Point: Bp₉ 184-187°

Aldrich: 28607-9

Fluka: 51640

Rare Chemicals Library: S56007-3

Sigma: H6757

Supelco: R42-0175

>>Derivative: Et ester

CAS Registry Number: 14010-23-2

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%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 28°

Boiling Point: Bp₅ 185°

Rare Chemicals Library: S43358-6

Sigma: H6629

>>Derivative: Chloride

CAS Registry Number: 40480-10-2

Molecular Formula: $\text{C}_{17}\text{H}_{33}\text{ClO}$

Molecular Weight: 288.9

Accurate Mass: 288.221992

Percentage Composition: C 70.68%; H 11.51%; Cl 12.27%; O 5.54%

Boiling Point: Bp₄ 176°

Density: d 0.88

Refractive Index: n_D²⁰ 1.4530