



>>Entry Name: Pentadecanoic acid

CAS Registry Number: 1002-84-2

$\text{H}_3\text{C}(\text{CH}_2)_{13}\text{COOH}$

Molecular Formula: $\text{C}_{15}\text{H}_{30}\text{O}_2$

Molecular Weight: 242.401

Accurate Mass: 242.22458

Percentage Composition: C 74.33%; H 12.47%; O 13.20%

Biological Source: Isol. from some plants, eg. bark of *Zanthoxylum carolinianum*. Occurs in lichens

Physical Description: Cryst. (Me_2CO aq.)

Melting Point: Mp 53°

Boiling Point: Bp₁₀₀ 257°. Bp_{0.05} 138-139°

Hazard & Toxicity: LD₅₀ (mus, ivn) 54 mg/kg ; BERDY HAZD : LD₅₀ (mus, ivn) 54 mg/kg

Aldrich: P360-0

Fluka: 76540

Sigma: P6125

>>Derivative: Me ester

CAS Registry Number: 7132-64-1

Molecular Formula: $\text{C}_{16}\text{H}_{32}\text{O}_2$

Molecular Weight: 256.428

Accurate Mass: 256.24023

Percentage Composition: C 74.94%; H 12.58%; O 12.48%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 18.5°

Aldrich: 23545-8

Fluka: 76560

Sigma: P6250

>>Derivative: Et ester

CAS Registry Number: 41114-00-5

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%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 14°

>>Derivative: Amide

CAS Registry Number: 3843-51-4

Molecular Formula: $\text{C}_{15}\text{H}_{31}\text{NO}$

Molecular Weight: 241.416

Accurate Mass: 241.240564

Percentage Composition: C 74.63%; H 12.94%; N 5.80%; O 6.63%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 103-104°

>>Derivative: Nitrile

Synonym(s): Pentadecanenitrile. 1-Cyanotetradecane

CAS Registry Number: 18300-91-9

Molecular Formula: $\text{C}_{15}\text{H}_{29}\text{N}$

Molecular Weight: 223.401

Accurate Mass: 223.229999

Percentage Composition: C 80.65%; H 13.08%; N 6.27%

Physical Description: Oil or solid

Melting Point: Mp 20-24°

Boiling Point: Bp₂₃ 181-185°

Refractive Index: n_D²⁵ 1.4413

Aldrich: 13763-4

Other: Riedel de Haën