



Formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>

MW: 256.43

CAS: 57-10-3

TNP NUMBER: TNP00434

MDL NUMBER: MFCD00002747

IUPAC: hexadecanoic acid

Smiles: CCCCCCCCCCCCCCCC(O)=O

Occurs as glyceryl ester in many oils and fats. Obtained from Plam oil.

REFERENCE: Merck 13, 7064 Bradley RL, et al. Dietary Fatty Acids Differentially Regulate Production of TNF-alpha and IL-10 by Murine 3T3-L1 Adipocytes. Obesity (Silver Spring). 2008 Feb 28

SOURCE: Occurs as the glyceryl ester in many oils and fats. Obtained from palm oil, Japan wax, or Chinese vegetable tallow

ACCEPTORS: 2

DONORS: 1

ROTATION BONDS: 15

N+O: 2

Chiral Centers: 0

LogP: 6.77

LogS: -5.2

LIPINSKI: 3

Monograph Number: 0007064

Title: Palmitic Acid

CAS Registry Number: 57-10-3

CAS Name: Hexadecanoic acid

Additional Names: hexadecylic acid; cetylic acid

Molecular Formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>

Molecular Weight: 256.42.

Percent Composition: C 74.94%, H 12.58%, O 12.48%

Line Formula: CH<sub>3</sub>(CH<sub>2</sub>)<sub>14</sub>COOH

Literature References: Occurs as the glyceryl ester in many oils and fats. Obtained from palm oil, Japan wax, or Chinese vegetable tallow. Purification: Magne et al., US 2791596 (1957 to Secretary of Agriculture). Toxicity study: L. Oro, A. Wretlind, Acta Pharmacol. Toxicol. 18, 141 (1961).

Properties: White, crystalline scales. d<sub>4</sub><sup>25</sup> 0.853. mp 63-64. bp<sub>15</sub> 215. n<sub>D</sub><sup>20</sup> 1.4273. Insol in water. Sparingly sol in cold alcohol or in petr ether; freely sol in hot alcohol, in ether, propyl alcohol, chloroform. LD<sub>50</sub> i.v. in mice: 57