



>>Entry Name: Octadecanedioic acid, 9CI

CAS Registry Number: 871-70-5

HOOC(CH₂)₁₆COOH

Molecular Formula: C₁₈H₃₄O₄

Molecular Weight: 314.464

Accurate Mass: 314.24571

Percentage Composition: C 68.75%; H 10.90%; O 20.35%

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 123-124°

>>Derivative: Di-Me ester

CAS Registry Number: 1472-93-1

Molecular Formula: C₂₀H₃₈O₄

Molecular Weight: 342.518

Accurate Mass: 342.27701

Percentage Composition: C 70.13%; H 11.18%; O 18.68%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 58-59°

Boiling Point: Bp₃ 205-207°

>>Derivative: Di-Et ester

CAS Registry Number: 1472-90-8

Molecular Formula: C₂₂H₄₂O₄

Molecular Weight: 370.571

Accurate Mass: 370.30831

Percentage Composition: C 71.31%; H 11.42%; O 17.27%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 48.2°

Boiling Point: Bp_{1.5} 201-204°

Rare Chemicals Library: S70706-6

>>Derivative: Dinitrile

Synonym(s): Octadecanedinitrile. 1,16-Dicyanohexadecane

CAS Registry Number: 7735-45-7

Molecular Formula: C₁₈H₃₂N₂

Molecular Weight: 276.464

Accurate Mass: 276.256548

Percentage Composition: C 78.20%; H 11.67%; N 10.13%

Physical Description: Wax or cryst. (EtOH)

Melting Point: Mp 58-59°

References:

Chuit, P., *Helv. Chim. Acta*, 1926, **9**, 264, (*synth, esters*)

Sengupta, A. *et al.*, *J. Indian Chem. Soc.*, 1956, **33**, 804, (*synth*)

Fujisawa, T. *et al.*, *Bull. Chem. Soc. Jpn.*, 1983, **56**, 345, (*synth*)

Cardinale, G. *et al.*, *Tetrahedron*, 1985, **41**, 2899; 6051, (*di-Me ester, synth*)

Pomonis, J.G., *Lipids*, 1990, **25**, 821, (*dinitrile, synth, ir, ms*)