



>>Entry Name: Hexadecanedioic acid, 9CI

Synonym(s): Thapsic acid

CAS Registry Number: 505-54-4

HOOC(CH₂)₁₄COOH

Molecular Formula: C₁₆H₃₀O₄

Molecular Weight: 286.411

Accurate Mass: 286.21441

Percentage Composition: C 67.10%; H 10.56%; O 22.34%

Biological Source: Occurs as esters in *Thapsia garganica* and in *Juniperus sabina*

Use/Importance: Several polyesters and polyamides have been synth.

Physical Description: Cryst. (EtOH or EtOAc)

Melting Point: Mp 126°

Aldrich: 17750-4

Fluka: 52230

Sigma: H8133

>>Derivative: Mono-Me ester

CAS Registry Number: 18451-85-9

Molecular Formula: C₁₇H₃₂O₄

Molecular Weight: 300.437

Accurate Mass: 300.23006

Percentage Composition: C 67.96%; H 10.74%; O 21.30%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 68.7-71.9° (45-46°)

>>Derivative: Di-Me ester

CAS Registry Number: 19102-90-0

Molecular Formula: C₁₈H₃₄O₄

Molecular Weight: 314.464

Accurate Mass: 314.24571

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

Melting Point: Mp 51-52°

Boiling Point: Bp_{0.3} 150-160°

>>Derivative: Mono-Et ester

CAS Registry Number: 18017-66-8

Molecular Formula: C₁₈H₃₄O₄

Molecular Weight: 314.464

Accurate Mass: 314.24571

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

Boiling Point: Bp₃ 220°

>>Derivative: Di-Et ester

CAS Registry Number: 15786-31-9

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.

Melting Point: Mp 39°

Boiling Point: Bp_{0.3} 160-165°