



>>Entry Name: Tridecanedioic acid

Synonym(s): Brassylic acid

CAS Registry Number: 505-52-2

HOOC(CH₂)₁₁COOH

Molecular Formula: C₁₃H₂₄O₄

Molecular Weight: 244.33

Accurate Mass: 244.16746

Percentage Composition: C 63.91%; H 9.90%; O 26.19%

Physical Description: Cryst. (EtOH aq. or EtOAc)

Melting Point: Mp 114° (111°)

Aldrich: U60-1

>>Derivative: Mono-Me ester

CAS Registry Number: 3927-59-1

Molecular Formula: C₁₄H₂₆O₄

Molecular Weight: 258.357

Accurate Mass: 258.18311

Percentage Composition: C 65.09%; H 10.14%; O 24.77%

Melting Point: Mp 58°

>>Derivative: Di-Me ester

CAS Registry Number: 1472-87-3

Molecular Formula: C₁₅H₂₈O₄

Molecular Weight: 272.384

Accurate Mass: 272.19876

Percentage Composition: C 66.14%; H 10.36%; O 23.50%

Melting Point: Mp 36°

Boiling Point: Bp 194°. Bp 326-328°

Aldrich: 17190-5

Rare Chemicals Library: S55780-3

>>Derivative: Di-Et ester

CAS Registry Number: 15423-05-9

Molecular Formula: C₁₇H₃₂O₄

Molecular Weight: 300.437

Accurate Mass: 300.23006

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

Melting Point: Mp 20°

Boiling Point: Bp₁₂ 204°

Rare Chemicals Library: S67728-0

>>Derivative: Et ester-chloride

Molecular Formula: C₁₅H₂₇ClO₃

Molecular Weight: 290.829

Accurate Mass: 290.164872

Percentage Composition: C 61.95%; H 9.36%; Cl 12.19%; O 16.50%

Boiling Point: Bp₅ 185-188°

>>Derivative: Et ester-amide

Molecular Formula: C₁₅H₂₉NO₃

Molecular Weight: 271.399

Accurate Mass: 271.214744

Percentage Composition: C 66.38%; H 10.77%; N 5.16%; O 17.69%

Melting Point: Mp 91-92°