



>>Derivative: Ac, Me ester

CAS Registry Number: 53562-87-1

Molecular Formula: C₇H₁₂O₄

Molecular Weight: 160.169

Accurate Mass: 160.07356

Percentage Composition: C 52.49%; H 7.55%; O 39.96%

Boiling Point: Bp₉ 75-76°

Optical Rotation: [α]_D²¹+0.5 (neat)

>>Variant: (±)-form

CAS Registry Number: 625-71-8

Molecular Formula: C₄H₈O₃

Molecular Weight: 104.105

Accurate Mass: 104.047345

Percentage Composition: C 46.15%; H 7.75%; O 46.11%

Physical Description: Hygroscopic syrup

Boiling Point: Bp₁₃ 130° (lit. gives a pressure range)

pKa Value: pK_a 4.29

Other Data: Steam-volatile

Sigma: H9256

>>Derivative: Na salt

CAS Registry Number: 306-31-0

Melting Point: Mp 165-167°

Fluka: 54965

Sigma: H6501

>>Derivative: Me ester

CAS Registry Number: 1487-49-6

Molecular Formula: C₅H₁₀O₃

Molecular Weight: 118.132

Accurate Mass: 118.062995

Percentage Composition: C 50.84%; H 8.53%; O 40.63%

Boiling Point: Bp_{12.5} 67-68° (lit. gives a pressure range)

Optical Rotation: [α]_D²⁵+33.3 (c, 1.2 in CHCl₃)

Hazard & Toxicity: Eye irritant

>>Derivative: Et ester

Synonym(s): FEMA 3428

CAS Registry Number: 35608-64-1

Extra CAS Registry Numbers(s): 5405-41-4

Molecular Formula: C₆H₁₂O₃

Molecular Weight: 132.159

Accurate Mass: 132.078645

Percentage Composition: C 54.53%; H 9.15%; O 36.32%

Boiling Point: Bp₈ 72-74°. Bp 184-185°

Density: d²⁵ 1.01

Refractive Index: n_D²⁰ 1.4200

>>Derivative: Amide

CAS Registry Number: 40482-53-9

Molecular Formula: C₄H₉NO₂

Molecular Weight: 103.121

Accurate Mass: 103.063329

Percentage Composition: C 46.59%; H 8.80%; N 13.58%; O 31.03%

Physical Description: Prisms (H₂O)

Melting Point: Mp 84-87°