



>>Derivative: Et ether, di-Me ester

Molecular Formula: C₈H₁₄O₅

Molecular Weight: 190.196

Accurate Mass: 190.084125

Percentage Composition: C 50.52%; H 7.42%; O 42.06%

Boiling Point: Bp₃₀ 121°

Optical Rotation: [α]_D¹³+59.86

Density: d₄¹³1.11

>>Variant: (S)-form

Synonym(s): L-form

CAS Registry Number: 97-67-6

Molecular Formula: C₄H₆O₅

Molecular Weight: 134.088

Accurate Mass: 134.021525

Percentage Composition: C 35.83%; H 4.51%; O 59.66%

Biological Source: Occurs naturally in apples and various other fruits

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 104-105° (100°)

Optical Rotation: [α]_D²¹−2.3 (c, 8.5 in H₂O). [α]_D²⁰−28.7 (c, 5.5 in Py) (>99.8% ee)

Solubility: V. sol. EtOH, spar. sol. Et₂O

pKa Value: pK_{a1} 3.46; pK_{a2} 5.1

Other Data: Dec. at *ca.* 140°. Specific rotn. concn. dependent. See (±)-form for food use

Aldrich: 11257-7

Fluka: 2290

Sigma: M7397

>>Derivative: 1-Me ester

CAS Registry Number: 66212-45-1

Molecular Formula: C₅H₈O₅

Molecular Weight: 148.115

Accurate Mass: 148.037175

Percentage Composition: C 40.55%; H 5.44%; O 54.01%

Melting Point: Mp 79-80°

Optical Rotation: [α]_D²⁰+5.8 (c, 9.5 in MeOH)

>>Derivative: 4-Me ester

CAS Registry Number: 66178-02-7

Molecular Formula: C₅H₈O₅

Molecular Weight: 148.115

Accurate Mass: 148.037175

Percentage Composition: C 40.55%; H 5.44%; O 54.01%

Optical Rotation: [α]_D +1.5 (c, 1.8 in CHCl₃)

>>Derivative: Di-Me ester

CAS Registry Number: 617-55-0

Molecular Formula: C₆H₁₀O₅

Molecular Weight: 162.142

Percentage Composition: C 44.45%; H 6.22%; O 49.34%

Physical Description: Oil

Boiling Point: Bp 242°. Bp₁₂ 122°

Optical Rotation: [α]_D²⁵−8.4 (pure liq.). [α]_D²⁰−10 (c, 2.2 in EtOH) (>99.8% ee)

Other Data: Prolonged heating leads to dimethyl fumarate. Easily dec. by H₂O

Aldrich: 37431-8

Fluka: 2315

>>Derivative: 1-Et ester