



Molecular Formula: C₉H₁₂O₄
Molecular Weight: 184.191
Accurate Mass: 184.07356
Percentage Composition: C 58.69%; H 6.57%; O 34.75%
Use/Importance: Chiral synthon obt. in opt. active form
Physical Description: Cryst. solid (Et₂O/hexane)
Melting Point: Mp 65.5-66°
Optical Rotation: [α]_D²⁰ +2.52 (c, 4.33 in CHCl₃)
Other Data: Props. refer to (1*R*,6*S*)-form

>>Derivative: Di-Me ester

CAS Registry Number: 69093-49-8
Molecular Formula: C₁₀H₁₄O₄
Molecular Weight: 198.218
Accurate Mass: 198.08921
Percentage Composition: C 60.59%; H 7.12%; O 32.29%
Melting Point: Mp 39-40°
UV: [neutral] $\lambda_{\max}$ 206 (ϵ 13940); 238 (ϵ 8960) (MeOH) (Derep)

>>Derivative: Anhydride

Physical Description: Cryst. (C₆H₆/petrol)
Melting Point: Mp 130° (141°)
Hazard & Toxicity: Eye, skin and mucous membrane irritant

>>Variant: (1*RS*,2*SR*)-form

Synonym(s): *cis*-form

CAS Registry Number: 2305-26-2
Molecular Formula: C₈H₁₀O₄
Molecular Weight: 170.165
Accurate Mass: 170.05791
Percentage Composition: C 56.47%; H 5.92%; O 37.61%
Physical Description: Prisms (H₂O)
Melting Point: Mp 174° (166°)
pKa Value: p*K*_{a1} 3.75; p*K*_{a2} 6.77 (25°)

>>Derivative: Mono-Me ester

CAS Registry Number: 31139-02-3
Molecular Formula: C₉H₁₂O₄
Molecular Weight: 184.191
Percentage Composition: C 58.69%; H 6.57%; O 34.75%
Source/Synthesis: Obt. on large scale in chiral form by pig-liver esterase hydrol. of the diester
Use/Importance: Chiral intermed. for synth.

>>Derivative: Di-Me ester

CAS Registry Number: 4841-84-3
Boiling Point: Bp₅ 110-111°
Aldrich: 34967-4

>>Derivative: Anhydride

Synonym(s): Tetrahydrophthalic anhydride

CAS Registry Number: 935-79-5
Use/Importance: Manuf. by Diels-Alder reaction of butadiene and maleic anhydride. Comonomer for unsatd. polyester resins. Epoxy resin curing agent
Physical Description: Cryst. (petrol)
Melting Point: Mp 103-104°
Solubility: Sol. C₆H₆; sl. sol. petrol, Et₂O
Hazard & Toxicity: Irritant
Aldrich: 13689-1
Fluka: 87460

References: