



CAS Registry Number: 19974-97-1
Molecular Formula: C₁₀H₁₆O₇
Molecular Weight: 248.232
Accurate Mass: 248.089605
Percentage Composition: C 48.39%; H 6.50%; O 45.12%
Physical Description: Needles (Et₂O)
Melting Point: Mp 58-59°
pKa Value: pK_a 3.28

>>Derivative: Tri-Et ester

CAS Registry Number: 77-93-0
Molecular Formula: C₁₂H₂₀O₇
Molecular Weight: 276.286
Accurate Mass: 276.120905
Percentage Composition: C 52.17%; H 7.30%; O 40.54%
Use/Importance: Plasticizer, sequestrant, pharmaceutical excipient
Physical Description: Oil
Boiling Point: Bp 294°. Bp₁ 127°
Solubility: Sl. sol. H₂O
Density: d²⁵ 1.136
Hazard & Toxicity: LD₅₀ (rat, orl) 5900 mg/kg

Aldrich: 10929-0
Fluka: 27500
Rare Chemicals Library: S41640-1

>>Derivative: Tributyl ester

CAS Registry Number: 77-94-1
Molecular Formula: C₁₈H₃₂O₇
Molecular Weight: 360.447
Accurate Mass: 360.214805
Percentage Composition: C 59.98%; H 8.95%; O 31.07%
Use/Importance: Plasticiser
Physical Description: Liq.
Boiling Point: Bp₃ 178-180°
Density: d²⁵ 1.042
Refractive Index: n_D²⁰ 1.4460
Rare Chemicals Library: S42932-5

>>Derivative: 2-*tert*-Butyl ester

CAS Registry Number: 114340-52-2
Molecular Formula: C₁₀H₁₆O₇
Molecular Weight: 248.232
Accurate Mass: 248.089605
Percentage Composition: C 48.39%; H 6.50%; O 45.12%
Physical Description: Cryst. (EtOAc/hexanes)
Melting Point: Mp 120-122°

>>Derivative: Tri-Ph ester

CAS Registry Number: 116557-40-5
Molecular Formula: C₂₄H₂₀O₇
Molecular Weight: 420.418
Accurate Mass: 420.120905
Percentage Composition: C 68.57%; H 4.79%; O 26.64%
Physical Description: Needles
Melting Point: Mp 124°
Solubility: Sol. hot EtOH; insol. H₂O