



Molecular Weight: 104.105
Accurate Mass: 104.047345
Percentage Composition: C 46.15%; H 7.75%; O 46.11%
Optical Rotation: $[\alpha]_D +10.3$ (c, 6 in H₂O)
Fluka: 54925
Sigma: H0390

>>Derivative: Na salt

CAS Registry Number: 127604-16-4
Physical Description: Cryst. (EtOH)
Melting Point: Mp 150-155°
Optical Rotation: $[\alpha]_D^{19} +11$ (c, 10 in H₂O)
Aldrich: 29837-9
Fluka: 54964

>>Derivative: Me ester

CAS Registry Number: 53562-86-0
Boiling Point: Bp₁₇ 71-73°
Optical Rotation: $[\alpha]_D^{23} +33.3$ (c, 1 in CHCl₃)
Aldrich: 24316-7
Fluka: 54958
Sigma: M1141

>>Derivative: Et ester

CAS Registry Number: 56816-01-4
Boiling Point: Bp 180-182°. Bp₃₀ 94-95°
Optical Rotation: $[\alpha]_D^{25} +43.9$ (c, 1.35 in CHCl₃)
Refractive Index: n_D²⁰ 1.4210
Aldrich: 37470-9
Fluka: 54955

>>Derivative: Et ester, *O*-β-D-glucopyranoside

Molecular Formula: C₁₂H₂₂O₈
Molecular Weight: 294.301
Accurate Mass: 294.13147
Percentage Composition: C 48.97%; H 7.53%; O 43.49%
Biological Source: Constit. of the fruit of *Carica pubescens*

>>Derivative: Butyl ester, *O*-β-D-glucopyranoside

Molecular Formula: C₁₄H₂₆O₈
Molecular Weight: 322.355
Accurate Mass: 322.16277
Percentage Composition: C 52.16%; H 8.13%; O 39.71%
Biological Source: Constit. of the fruit of *Carica pubescens*

>>Derivative: Nitrile

CAS Registry Number: 123689-95-2
Molecular Formula: C₄H₇NO
Molecular Weight: 85.105
Accurate Mass: 85.052764
Percentage Composition: C 56.45%; H 8.29%; N 16.46%; O 18.80%
Boiling Point: Bp₁₅ 99-100°
Optical Rotation: $[\alpha]_D^{18} +8.78$

>>Derivative: Ac

CAS Registry Number: 25654-45-9
Molecular Formula: C₆H₁₀O₄
Molecular Weight: 146.143
Accurate Mass: 146.05791
Percentage Composition: C 49.31%; H 6.90%; O 43.79%
Optical Rotation: $[\alpha]$