



CAS Registry Number: 86491-59-0

Molecular Formula: C₁₆H₂₈O₁₁

Molecular Weight: 396.391

Accurate Mass: 396.163165

Percentage Composition: C 48.48%; H 7.12%; O 44.40%

Biological Source: Isol. from immature pods of *Acacia sieberiana* var. *woodii*

Melting Point: Mp 147-148.5° (as hexa-Ac)

Optical Rotation: [α]_D²⁰+8.5 (c, 0.46 in CHCl₃) (hexa-Ac)

>>Derivative: Chloride

CAS Registry Number: 27763-54-8

Extra CAS Registry Numbers(s): 5856-79-1

Molecular Formula: C₅H₉ClO

Molecular Weight: 120.578

Accurate Mass: 120.034192

Percentage Composition: C 49.81%; H 7.52%; Cl 29.40%; O 13.27%

Boiling Point: Bp 119-120°

Optical Rotation: [α]_D²⁵+19.2 (H₂O)

>>Derivative: Amide

CAS Registry Number: 13133-74-9

Molecular Formula: C₅H₁₁NO

Molecular Weight: 101.148

Accurate Mass: 101.084064

Percentage Composition: C 59.37%; H 10.96%; N 13.85%; O 15.82%

Physical Description: Cryst.

Melting Point: Mp 111°

Optical Rotation: [α]_D²⁵+22.4

>>Derivative: Nitrile

Synonym(s): 2-Cyanobutane

CAS Registry Number: 25570-03-0

Molecular Formula: C₅H₉N

Molecular Weight: 83.133

Accurate Mass: 83.073499

Percentage Composition: C 72.24%; H 10.91%; N 16.85%

Boiling Point: Bp 125-126°

Aldrich: 24730-8

Sigma: M0641

>>Derivative: Anhydride

CAS Registry Number: 84131-91-9

Molecular Formula: C₁₀H₁₈O₃

Molecular Weight: 186.25

Accurate Mass: 186.125595

Percentage Composition: C 64.49%; H 9.74%; O 25.77%

Boiling Point: Bp_{0.2} 66°

Optical Rotation: [α]_D²⁰+35 (neat)

Refractive Index: n_D²⁰ 1.4180

Aldrich: 34856-2

>>Variant: (±)-form

CAS Registry Number: 600-07-7

Molecular Formula: C₅H₁₀O₂

Molecular Weight: 102.133

Accurate Mass: 102.06808

Percentage Composition: C 58.80%; H 9.87%; O 31.33%

Physical Description: Liq. with fruity taste at low concentrations

Boiling Point: Bp 177°. Bp₂₁ 84°