



**CAS Registry Number:** 86491-59-0

**Molecular Formula:**  $C_{16}H_{28}O_{11}$

**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:**  $[\alpha]_D^{20} +8.5$  (c, 0.46 in  $CHCl_3$ ) (hexa-Ac)

>>Derivative: Chloride

**CAS Registry Number:** 27763-54-8

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

**Molecular Formula:**  $C_5H_9ClO$

**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:**  $[\alpha]_D^{25} +19.2$  ( $H_2O$ )

>>Derivative: Amide

**CAS Registry Number:** 13133-74-9

**Molecular Formula:**  $C_5H_{11}NO$

**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:**  $[\alpha]_D^{25} +22.4$

>>Derivative: Nitrile

**Synonym(s):** 2-Cyanobutane

**CAS Registry Number:** 25570-03-0

**Molecular Formula:**  $C_5H_9N$

**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:**  $C_{10}H_{18}O_3$

**Molecular Weight:** 186.25

**Accurate Mass:** 186.125595

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

**Boiling Point:** Bp<sub>0.2</sub> 66°

**Optical Rotation:**  $[\alpha]_D^{20} +35$  (neat)

**Refractive Index:**  $n_D^{20}$  1.4180

**Aldrich:** 34856-2

>>Variant: (±)-form

**CAS Registry Number:** 600-07-7

**Molecular Formula:**  $C_5H_{10}O_2$

**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°. Bp<sub>21</sub> 84°