



Aldrich: 34895-3

>> **Derivative:** 1-Methylheptyl ester

CAS Registry Number: 52688-08-1

Molecular Formula: C₁₁H₁₉NO₂

Molecular Weight: 197.277

Accurate Mass: 197.141579

Percentage Composition: C 66.97%; H 9.71%; N 7.10%; O 16.22%

Boiling Point: Bp₇ 142°

Other: Hüls

>> **Derivative:** 2-Methoxy-1-methylethyl ester

CAS Registry Number: 32804-79-8

Molecular Formula: C₇H₁₁NO₃

Molecular Weight: 157.169

Accurate Mass: 157.073894

Percentage Composition: C 53.49%; H 7.05%; N 8.91%; O 30.54%

Boiling Point: Bp₅ 115°

Aldrich: 41146-9

Other: Hüls

>> **Derivative:** 2-Methoxyethyl ester

CAS Registry Number: 10258-54-5

Molecular Formula: C₆H₉NO₃

Molecular Weight: 143.142

Accurate Mass: 143.058244

Percentage Composition: C 50.35%; H 6.34%; N 9.79%; O 33.53%

Boiling Point: Bp_{0.8} 95-98°

Aldrich: 41147-7

Other: Hüls

>> **Derivative:** 2-Ethoxyethyl ester

CAS Registry Number: 32804-77-6

Molecular Formula: C₇H₁₁NO₃

Molecular Weight: 157.169

Accurate Mass: 157.073894

Percentage Composition: C 53.49%; H 7.05%; N 8.91%; O 30.54%

Boiling Point: Bp_{0.3} 104-108°

Other: Hüls

>> **Derivative:** Amide

Synonym(s): Cyanoacetamide. Malonic amide nitrile

CAS Registry Number: 107-91-5

Molecular Formula: C₃H₄N₂O

Molecular Weight: 84.077

Accurate Mass: 84.032363

Percentage Composition: C 42.86%; H 4.80%; N 33.32%; O 19.03%

Use/Importance: Anal. reagent for carbohydrates

Melting Point: Mp 119-120°

Solubility: Sol. H₂O, mod. sol. EtOH

Hazard & Toxicity: LD₅₀ (rat, orl) 7230 mg/kg

Aldrich: 10844-8

Fluka: 28280