



Density: d_4^{20} 1.01
Fluka: 28452
Rare Chemicals Library: S61513-7
Other: Hüls

>> **Derivative:** 2-Propenyl ester
Synonym(s): Allyl cyanoacetate

CAS Registry Number: 13361-32-5
Molecular Formula: $C_6H_7NO_2$
Molecular Weight: 125.127
Accurate Mass: 125.047679
Percentage Composition: C 57.59%; H 5.64%; N 11.19%; O 25.57%
Boiling Point: Bp_{20} 110°
Density: d 1.06
Refractive Index: n_D^{20} 1.4430

>> **Derivative:** Butyl ester

CAS Registry Number: 5459-58-5
Molecular Formula: $C_7H_{11}NO_2$
Molecular Weight: 141.169
Accurate Mass: 141.078979
Percentage Composition: C 59.56%; H 7.85%; N 9.92%; O 22.67%
Boiling Point: Bp_{15} 115°
Refractive Index: n_D^{20} 1.4250

Aldrich: 24570-4
Rare Chemicals Library: S54971-1

>> **Derivative:** 2-Methylpropyl ester

CAS Registry Number: 13361-31-4
Molecular Formula: $C_7H_{11}NO_2$
Molecular Weight: 141.169
Accurate Mass: 141.078979
Percentage Composition: C 59.56%; H 7.85%; N 9.92%; O 22.67%
Boiling Point: Bp 223°
Density: d_4^{20} 0.99
Other: Hüls

>> **Derivative:** *tert*-Butyl ester
Synonym(s): *tert*-Butyl cyanoacetate

CAS Registry Number: 1116-98-9
Molecular Formula: $C_7H_{11}NO_2$
Molecular Weight: 141.169
Accurate Mass: 141.078979
Percentage Composition: C 59.56%; H 7.85%; N 9.92%; O 22.67%
Use/Importance: Condensing agent with some advantages over the Et ester
Boiling Point: $Bp_{1.5}$ 67-68°

>> **Derivative:** 2-Ethylhexyl ester

CAS Registry Number: 13361-34-7
Molecular Formula: $C_{11}H_{19}NO_2$
Molecular Weight: 197.277
Accurate Mass: 197.141579
Percentage Composition: C 66.97%; H 9.71%; N 7.10%; O 16.22%
Boiling Point: Bp_{11} 148-159°. Bp_5 140°
Aldrich: 10839-1
Fluka: 28445
Rare Chemicals Library: S43143-5
Other: Hüls

>> **Derivative:** Octyl ester

CAS Registry Number: 15666-97-4
Boiling Point: Bp_6 144°. $Bp_{0.11}$ 95°
Refractive Index: n