



>>Entry Name: Cyanoacetic acid, 9CI

Synonym(s): Malonic acid mononitrile

CAS Registry Number: 372-09-8

NCCH<sub>2</sub>COOH

Molecular Formula: C<sub>3</sub>H<sub>3</sub>NO<sub>2</sub>

Molecular Weight: 85.062

Accurate Mass: 85.016379

Percentage Composition: C 42.36%; H 3.55%; N 16.47%; O 37.62%

Melting Point: Mp 66°

Boiling Point: Bp 108°

Solubility: Sol. H<sub>2</sub>O, EtOH, Et<sub>2</sub>O

pKa Value: pK<sub>a</sub> 2.43 (25°)

Hazard & Toxicity: Explosive reaction with furfuryl alcohol when heated. LD<sub>50</sub> (rat, orl) 1500 mg/kg

Aldrich: 23997-6

Fluka: 28410

Sigma: C5140

>>Derivative: Me ester

Synonym(s): Methyl cyanoacetate

CAS Registry Number: 105-34-0

Molecular Formula: C<sub>4</sub>H<sub>5</sub>NO<sub>2</sub>

Molecular Weight: 99.089

Accurate Mass: 99.032029

Percentage Composition: C 48.49%; H 5.09%; N 14.14%; O 32.29%

Boiling Point: Bp 200°. Bp<sub>36</sub> 115°

Hazard & Toxicity: Fl. p. 103°

Aldrich: 10842-1

Fluka: 28460

>>Derivative: Et ester

Synonym(s): Ethyl cyanoacetate

CAS Registry Number: 105-56-6

Molecular Formula: C<sub>5</sub>H<sub>7</sub>NO<sub>2</sub>

Molecular Weight: 113.116

Accurate Mass: 113.047679

Percentage Composition: C 53.09%; H 6.24%; N 12.38%; O 28.29%

Use/Importance: Reagent for condensations

Boiling Point: Bp 207°. Bp<sub>16</sub> 97°

Solubility: Insol. H<sub>2</sub>O; sol. NH<sub>3</sub> aq.

Hazard & Toxicity: Fl. p. 104/110°

Aldrich: E1842-5

Fluka: 28429

>>Derivative: Propyl ester

CAS Registry Number: 14447-15-5

Molecular Formula: C<sub>6</sub>H<sub>9</sub>NO<sub>2</sub>

Molecular Weight: 127.143

Accurate Mass: 127.063329

Percentage Composition: C 56.68%; H 7.13%; N 11.02%; O 25.17%

Boiling Point: Bp 216°

Density: d<sub>4</sub><sup>20</sup> 1.02

Other: Hüls