



>>Entry Name: Isocyanatoacetic acid, 9CI

Synonym(s): Carbonylglycine

CAS Registry Number: 65461-92-9

OCNCH<sub>2</sub>COOH

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

Molecular Weight: 101.062

Accurate Mass: 101.011294

Percentage Composition: C 35.65%; H 2.99%; N 13.86%; O 47.49%

>>Derivative: Me ester

CAS Registry Number: 30988-17-1

Molecular Formula: C<sub>4</sub>H<sub>5</sub>NO<sub>3</sub>

Molecular Weight: 115.088

Accurate Mass: 115.026944

Percentage Composition: C 41.75%; H 4.38%; N 12.17%; O 41.71%

Physical Description: Liq.

Boiling Point: Bp<sub>19</sub> 73°

>>Derivative: Et ester

CAS Registry Number: 2949-22-6

Molecular Formula: C<sub>5</sub>H<sub>7</sub>NO<sub>3</sub>

Molecular Weight: 129.115

Accurate Mass: 129.042594

Percentage Composition: C 46.51%; H 5.46%; N 10.85%; O 37.17%

Physical Description: Liq.

Boiling Point: Bp<sub>11</sub> 67-68°

Refractive Index: n<sub>D</sub><sup>20</sup> 1.4220

Aldrich: 23862-7

Fluka: 58808

>>Derivative: Benzyl ester

Molecular Formula: C<sub>10</sub>H<sub>9</sub>NO<sub>3</sub>

Molecular Weight: 191.186

Accurate Mass: 191.058244

Percentage Composition: C 62.82%; H 4.74%; N 7.33%; O 25.11%

Boiling Point: Bp<sub>0.5</sub> 120°

>>Derivative: Chloride

CAS Registry Number: 2185-10-6

Molecular Formula: C<sub>3</sub>H<sub>2</sub>ClNO<sub>2</sub>

Molecular Weight: 119.507

Accurate Mass: 118.977406

Percentage Composition: C 30.15%; H 1.69%; Cl 29.67%; N 11.72%; O 26.78%

Physical Description: Liq.

Boiling Point: Bp<sub>45</sub> 71-72°

>>Derivative: Nitrile

#### References:

*Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **1**, 1407C, (*nmr*)

*Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 872C, (*ir*)

*Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 824C, (*ir*)

Benn, M.H. *et al.*, *J.C.S.*, 1961, 2365, (*Me ester*)

Elderfield, R.C. *et al.*, *J.O.C.*, 1961, **26**, 1917, (*Et ester*)

Mormann, W. *et al.*, *Chem. Ber.*, 1987, **120**, 285, (*chloride*)

Ono, N. *et al.*, *J. Het. Chem.*, 1994, **31**, 707, (*benzyl ester*)