



>>Entry Name: 5-Isoxazolecarboxylic acid

CAS Registry Number: 21169-71-1

Molecular Formula:  $C_4H_3NO_3$

Molecular Weight: 113.073

Accurate Mass: 113.011294

Percentage Composition: C 42.49%; H 2.67%; N 12.39%; O 42.45%

Physical Description: Pale-yellow cryst.

Melting Point: Mp 149 subl.°

>>Derivative: Me ester

CAS Registry Number: 15055-81-9

Molecular Formula:  $C_5H_5NO_3$

Molecular Weight: 127.099

Accurate Mass: 127.026944

Percentage Composition: C 47.25%; H 3.97%; N 11.02%; O 37.76%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 49-50°

Boiling Point: Bp<sub>12</sub> 100-101°

>>Derivative: Et ester

Molecular Formula:  $C_6H_7NO_3$

Molecular Weight: 141.126

Accurate Mass: 141.042594

Percentage Composition: C 51.06%; H 5.00%; N 9.92%; O 34.01%

Physical Description: Oil

Boiling Point: Bp<sub>1</sub> 110°

>>Derivative: Amide

Molecular Formula:  $C_4H_4N_2O_2$

Molecular Weight: 112.088

Accurate Mass: 112.027278

Percentage Composition: C 42.86%; H 3.60%; N 24.99%; O 28.55%

Melting Point: Mp 173-174°

>>Derivative: Nitrile

Synonym(s): 5-Cyanoisoxazole

CAS Registry Number: 68776-59-0

Molecular Formula:  $C_4H_2N_2O$

Molecular Weight: 94.073

Accurate Mass: 94.016713

Percentage Composition: C 51.07%; H 2.14%; N 29.78%; O 17.01%

Physical Description: Oil

Boiling Point: Bp 168°

>>Derivative: Chloride

CAS Registry Number: 62348-13-4

Molecular Formula:  $C_4H_2ClNO_2$

Molecular Weight: 131.518

Accurate Mass: 130.977406

Percentage Composition: C 36.53%; H 1.53%; Cl 26.96%; N 10.65%; O 24.33%

Physical Description: Liq.

Boiling Point: Bp<sub>20</sub> 74-76°

References:

Quilico, A. *et al.*, *Gazz. Chim. Ital.*, 1949, **79**, 654, (*synth*)

Spiegler, W. *et al.*, *Synthesis*, 1986, 69, (*synth, deriv, ir, pmr*)