



>>Entry Name: 4-Oxazolecarboxylic acid, 9CI

CAS Registry Number: 23012-13-7

Related CAS Registry Numbers(s): 62348-20-3

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: Solid (EtOH/ $C_6H_6$ )

Melting Point: Mp 100° (hydrate). Mp 142°

pKa Value:  $pK_a$  3.41 (20°,  $H_2O$ )

>>Derivative: Et ester

CAS Registry Number: 23012-14-8

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: Prisms ( $C_6H_6$ /petrol)

Melting Point: Mp 47-49°

Boiling Point: Bp<sub>14</sub> 101-102°. Bp<sub>3</sub> 63-67°

>>Derivative: Amide

CAS Registry Number: 23012-15-9

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%

Physical Description: Needles (MeOH)

Melting Point: Mp 161-162°

>>Derivative: Nitrile

Synonym(s): 4-Cyanooxazole

CAS Registry Number: 55242-84-7

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%

Boiling Point: Bp<sub>15</sub> 70-90°

#### References:

Cornforth, J.W. *et al.*, *J.C.S.*, 1947, 96, (*synth*)

Rinderspacher, T. *et al.*, *Helv. Chim. Acta*, 1960, **43**, 1522, (*amide, nitrile*)

Brown, D.J. *et al.*, *J.C.S.(B)*, 1969, 270, (*pmr*)

Henneke, K.W. *et al.*, *Annalen*, 1979, 1370, (*synth, pmr, ir*)