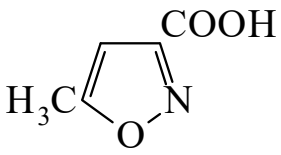
>>**Entry Name: 5-Methyl-3-isoxazolecarboxylic acid,** 9CI



CAS Registry Number: 3405-77-4

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: Prisms or plates (H_2O)
Melting Point: Mp 176°

>>**Derivative:** Me ester
Synonym(s): Premnazole

CAS Registry Number: 19788-35-3

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%
Biological Source: Constit. of the leaves of *Gmelina arborea* and *Premna integrifolia*
Biological Use/Importance: Antiinflammatory
Physical Description: Cryst. (C_6H_6)
Melting Point: Mp 98-99°

>>**Derivative:** Et ester

CAS Registry Number: 3209-72-1
Molecular Formula: $C_7H_9NO_3$
Molecular Weight: 155.153
Accurate Mass: 155.058244
Percentage Composition: C 54.19%; H 5.85%; N 9.03%; O 30.94%
Boiling Point: Bp_{15} 140°

>>**Derivative:** Amide

CAS Registry Number: 3445-52-1
Molecular Formula: $C_5H_6N_2O_2$
Molecular Weight: 126.115
Accurate Mass: 126.042928
Percentage Composition: C 47.62%; H 4.80%; N 22.21%; O 25.37%
Melting Point: Mp 166°

>>**Derivative:** Nitrile
Synonym(s): 3-Cyano-5-methylisoxazole

CAS Registry Number: 57351-99-2
Molecular Formula: $C_5H_4N_2O$
Molecular Weight: 108.099
Accurate Mass: 108.032363
Percentage Composition: C 55.56%; H 3.73%; N 25.91%; O 14.80%
Boiling Point: Bp_{25} 87-88°

References:

Good, R.H. *et al.*, *J.C.S. Perkin 1*, 1972, 2441
Barik, B.R. *et al.*, *Fitoterapia*, 1992, **63**, 295, *(Premnazole)*
Khanna, I.K. *et al.*, *J. Med. Chem.*, 2000, **43**, 3168-3185, *(nitrile, synth, pmr)*