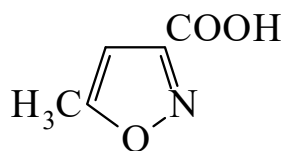




>>Entry Name: 5-Methyl-3-isoxazolecarboxylic acid, 9CI



CAS Registry Number: 3405-77-4

Molecular Formula: C₅H₅NO₃

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 (H₂O)

Melting Point: Mp 176°

>>Derivative: Me ester

Synonym(s): Premnazole

CAS Registry Number: 19788-35-3

Molecular Formula: C₆H₇NO₃

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. (C₆H₆)

Melting Point: Mp 98-99°

>>Derivative: Et ester

CAS Registry Number: 3209-72-1

Molecular Formula: C₇H₉NO₃

Molecular Weight: 155.153

Accurate Mass: 155.058244

Percentage Composition: C 54.19%; H 5.85%; N 9.03%; O 30.94%

Boiling Point: Bp₁₅ 140°

>>Derivative: Amide

CAS Registry Number: 3445-52-1

Molecular Formula: C₅H₆N₂O₂

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: C₅H₄N₂O

Molecular Weight: 108.099

Accurate Mass: 108.032363

Percentage Composition: C 55.56%; H 3.73%; N 25.91%; O 14.80%

Boiling Point: Bp₂₅ 87-88°

References:

Good, R.H. *et al.*, *J.C.S. Perkin I*, 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*)