



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

CAS Registry Number: 4857-42-5

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%

Melting Point: Mp 211°

>>Derivative: Me 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: Granular cryst. solid

Melting Point: Mp 108°

Other Data: Incorrectly named in the paper

>>Derivative: Et ester

CAS Registry Number: 63366-79-0

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%

Melting Point: Mp 27°

Boiling Point: Bp₂₀ 119°

>>Derivative: Chloride

CAS Registry Number: 49783-72-4

Molecular Formula: $C_5H_4ClNO_2$

Molecular Weight: 145.545

Accurate Mass: 144.993056

Percentage Composition: C 41.26%; H 2.77%; Cl 24.36%; N 9.62%; O 21.99%

Melting Point: Mp 39°

Boiling Point: Bp₂₀ 89°

References:

Casnati, G. *et al.*, *Tet. Lett.*, 1967, 327

Bell, D. *et al.*, *Tetrahedron*, 1994, **50**, 6643, (*Me ester*)