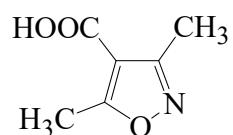




>>Entry Name: 3,5-Dimethyl-4-isoxazolecarboxylic acid, 9CI



CAS Registry Number: 2510-36-3

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%

Physical Description: Cryst. (H₂O or C₆H₆)

Melting Point: Mp 141-142°

>>Derivative: Et ester

CAS Registry Number: 17147-42-1

Molecular Formula: C₈H₁₁NO₃

Molecular Weight: 169.18

Accurate Mass: 169.073894

Percentage Composition: C 56.80%; H 6.55%; N 8.28%; O 28.37%

Physical Description: Oil

Boiling Point: Bp_{0.5} 60-63°

>>Derivative: Amide

Molecular Formula: C₆H₈N₂O₂

Molecular Weight: 140.141

Accurate Mass: 140.058578

Percentage Composition: C 51.42%; H 5.75%; N 19.99%; O 22.83%

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 149°

>>Derivative: Nitrile

Synonym(s): 4-Cyano-3,5-dimethylisoxazole

CAS Registry Number: 31301-46-9

Molecular Formula: C₆H₆N₂O

Molecular Weight: 122.126

Accurate Mass: 122.048013

Percentage Composition: C 59.01%; H 4.95%; N 22.94%; O 13.10%

Physical Description: Volatile plates with unpleasant odour

Melting Point: Mp 45-46°

Boiling Point: Bp₃₀ 110-112°

References:

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- Stork, G. *et al.*, *J.A.C.S.*, 1967, **89**, 5461-5462, (*synth, Et ester, pmr*)
- Bowles, K.D. *et al.*, *J. Chem. Educ.*, 1985, **62**, 1118-1120, (*synth, Et ester, pmr, ir, ms*)
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