



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

CAS Registry Number: 14442-12-7

Molecular Formula: $C_{10}H_7NO_3$

Molecular Weight: 189.17

Accurate Mass: 189.042594

Percentage Composition: C 63.49%; H 3.73%; N 7.40%; O 25.37%

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 181-182°

>>Derivative: Me ester

CAS Registry Number: 1081-30-7

Molecular Formula: $C_{11}H_9NO_3$

Molecular Weight: 203.197

Accurate Mass: 203.058244

Percentage Composition: C 65.02%; H 4.46%; N 6.89%; O 23.62%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 108-109°

>>Derivative: Nitrile

Synonym(s): 5-Cyano-3-phenylisoxazole

CAS Registry Number: 1011-39-8

Molecular Formula: $C_{10}H_6N_2O$

Molecular Weight: 170.17

Accurate Mass: 170.048013

Percentage Composition: C 70.58%; H 3.55%; N 16.46%; O 9.40%

Physical Description: Solid (hexane)

Melting Point: Mp 88-89°

References:

Quilico, A. *et al.*, *Gazz. Chim. Ital.*, 1946, **76**, 148-166, (*synth*)

Stagno d'Alcontres, G. *et al.*, *Gazz. Chim. Ital.*, 1960, **90**, 1239-1252, (*synth*)

Christl, M. *et al.*, *Chem. Ber.*, 1973, **106**, 3275-3290, (*synth*)

Yedidia, V. *et al.*, *Can. J. Chem.*, 1980, **58**, 1144-1150, (*Me ester*)