



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

CAS Registry Number: 14441-90-8

Molecular Formula: C₁₀H₇NO₃

Molecular Weight: 189.17

Accurate Mass: 189.042594

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

Physical Description: Needles (H₂O)

Melting Point: Mp 160°

>>Derivative: Me ester

CAS Registry Number: 51677-09-9

Molecular Formula: C₁₁H₉NO₃

Molecular Weight: 203.197

Accurate Mass: 203.058244

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

Physical Description: Plates

Melting Point: Mp 87°

>>Derivative: Et ester

CAS Registry Number: 7063-99-2

Molecular Formula: C₁₂H₁₁NO₃

Molecular Weight: 217.224

Accurate Mass: 217.073894

Percentage Composition: C 66.35%; H 5.10%; N 6.45%; O 22.10%

Melting Point: Mp 55-57°

>>Derivative: Nitrile

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

CAS Registry Number: 14442-24-1

Molecular Formula: C₁₀H₆N₂O

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 (petrol)

Melting Point: Mp 88-89°

References:

- Quilico, A. *et al.*, *Gazz. Chim. Ital.*, 1949, **79**, 703-708, (*synth*)
Vaughan, W.R. *et al.*, *J.O.C.*, 1960, **25**, 1160-1164, (*synth*)
Grundmann, C. *et al.*, *J.O.C.*, 1966, **31**, 4235-4237, (*nitrile*)
Ger. Pat., 1971, 2 062 373; *CA*, **75**, 88597g, (*synth*)
King, G.S. *et al.*, *J.C.S. Perkin 1*, 1972, 437-443, (*synth*)
Dannhardt, G. *et al.*, *Arch. Pharm. (Weinheim, Ger.)*, 1995, **328**, 437-443, (*Me ester*)