



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

CAS Registry Number: 1136-45-4

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: Needles

Melting Point: Mp 191-193°

Hazard & Toxicity: LD₅₀ (rat, ipr) 1500 mg/kg

>>Derivative: Me ester

CAS Registry Number: 2065-28-3

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%

Physical Description: Cryst.

Melting Point: Mp 79-80°

>>Derivative: Et ester

CAS Registry Number: 1143-82-4

Molecular Formula: C₁₃H₁₃NO₃

Molecular Weight: 231.251

Accurate Mass: 231.089544

Percentage Composition: C 67.52%; H 5.67%; N 6.06%; O 20.76%

Physical Description: Cryst.

Melting Point: Mp 49°

>>Derivative: Methanamide

Synonym(s): N,5-Dimethyl-3-phenyl-4-isoxazolecarboxamide, 9CI

CAS Registry Number: 60986-88-1

Molecular Formula: C₁₂H₁₂N₂O₂

Molecular Weight: 216.239

Accurate Mass: 216.089878

Percentage Composition: C 66.65%; H 5.59%; N 12.95%; O 14.80%

Melting Point: Mp 154-156°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 636C, (ir)

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 505A, (nmr)

Adachi, I. *et al.*, *Chem. Pharm. Bull.*, 1968, **16**, 117, (synth)

Christl, M. *et al.*, *Chem. Ber.*, 1973, **106**, 3275, (synth, ir, pmr)

Dietliker, K. *et al.*, *Helv. Chim. Acta*, 1976, **59**, 2074, (synth, ir, uv, pmr)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, MNV000