



>>Entry Name: **5-Amino-3-phenylisoxazole**

Synonym(s): 3-Phenyl-5-isoxazamine

CAS Registry Number: 4369-55-5

Molecular Formula: $C_9H_8N_2O$

Molecular Weight: 160.175

Accurate Mass: 160.063663

Percentage Composition: C 67.49%; H 5.03%; N 17.49%; O 9.99%

Physical Description: Cryst.

Melting Point: Mp 110-112°

>>Derivative: *N*-Formyl

CAS Registry Number: 86685-13-4

Molecular Formula: $C_{10}H_8N_2O_2$

Molecular Weight: 188.185

Accurate Mass: 188.058578

Percentage Composition: C 63.83%; H 4.28%; N 14.89%; O 17.00%

Physical Description: Cryst. + $\frac{1}{2}$ H₂O (H₂O)

Melting Point: Mp 115-117° (112°)

>>Derivative: *N*-Ac

CAS Registry Number: 31301-40-3

Molecular Formula: $C_{11}H_{10}N_2O_2$

Molecular Weight: 202.212

Accurate Mass: 202.074228

Percentage Composition: C 65.34%; H 4.98%; N 13.85%; O 15.82%

Physical Description: Cryst.

Melting Point: Mp 163-164°

>>Derivative: *N*-Me

CAS Registry Number: 86685-14-5

Molecular Formula: $C_{10}H_{10}N_2O$

Molecular Weight: 174.202

Accurate Mass: 174.079313

Percentage Composition: C 68.95%; H 5.79%; N 16.08%; O 9.18%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 110-112°

>>Derivative: *N*-Et

CAS Registry Number: 86685-93-0

Molecular Formula: $C_{11}H_{12}N_2O$

Molecular Weight: 188.229

Accurate Mass: 188.094963

Percentage Composition: C 70.19%; H 6.43%; N 14.88%; O 8.50%

Physical Description: Cryst. (hexane/toluene)

Melting Point: Mp 115-116°

>>Derivative: *N*-Ph

CAS Registry Number: 15055-49-9

Molecular Formula: $C_{15}H_{12}N_2O$

Molecular Weight: 236.273

Accurate Mass: 236.094963

Percentage Composition: C 76.25%; H 5.12%; N 11.86%; O 6.77%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 143-144° (131-133°)

References:

Boulton, A.J. *et al.*, *Tetrahedron*, 1961, **17**, 51, (*ir, uv, struct*)

Iwai, I. *et al.*, *Chem. Pharm. Bull.*, 1966, **14**, 1277, (*synth, pmr*)

Griss, G. *et al.*, *Annalen*, 1970, **738**, 60, (*synth*)

Tatee, T. *et al.*, *Chem. Pharm. Bull.*, 1986, **34**, 1643, (*derivs*)