



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

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

CAS Registry Number: 4369-55-5

Molecular Formula: C<sub>9</sub>H<sub>8</sub>N<sub>2</sub>O

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<sub>10</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>

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. + ½ H<sub>2</sub>O (H<sub>2</sub>O)

Melting Point: Mp 115-117° (112°)

>>Derivative: N-Ac

CAS Registry Number: 31301-40-3

Molecular Formula: C<sub>11</sub>H<sub>10</sub>N<sub>2</sub>O<sub>2</sub>

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<sub>10</sub>H<sub>10</sub>N<sub>2</sub>O

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. (C<sub>6</sub>H<sub>6</sub>)

Melting Point: Mp 110-112°

>>Derivative: N-Et

CAS Registry Number: 86685-93-0

Molecular Formula: C<sub>11</sub>H<sub>12</sub>N<sub>2</sub>O

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<sub>15</sub>H<sub>12</sub>N<sub>2</sub>O

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