



>>Variant: (ξ)-form

**Molecular Formula:** C<sub>4</sub>H<sub>7</sub>NO<sub>2</sub>

**Molecular Weight:** 101.105

**Accurate Mass:** 101.047679

**Percentage Composition:** C 47.52%; H 6.98%; N 13.85%; O 31.65%

>>Derivative: Me ester

**CAS Registry Number:** 14205-39-1

**Molecular Formula:** C<sub>5</sub>H<sub>9</sub>NO<sub>2</sub>

**Molecular Weight:** 115.132

**Accurate Mass:** 115.063329

**Percentage Composition:** C 52.16%; H 7.88%; N 12.17%; O 27.79%

**Physical Description:** Prisms

**Melting Point:** Mp 85 subl.°

**Other Data:** Config. of this ester not detd.

**Aldrich:** 12971-2

**Fluka:** 7590

**Rare Chemicals Library:** S61388-6

**Sigma:** M9521

>>Derivative: Et ester

**CAS Registry Number:** 626-34-6

**Extra CAS Registry Numbers(s):** 7318-00-5

**Molecular Formula:** C<sub>6</sub>H<sub>11</sub>NO<sub>2</sub>

**Molecular Weight:** 129.158

**Accurate Mass:** 129.078979

**Percentage Composition:** C 55.80%; H 8.58%; N 10.84%; O 24.77%

**Melting Point:** Mp 33-35°

**Boiling Point:** Bp 210-215°

**Aldrich:** E1080-7

>>Derivative: Isopropyl ester

**CAS Registry Number:** 14205-46-0

**Extra CAS Registry Numbers(s):** 40100-28-5 143093-33-8

**Molecular Formula:** C<sub>7</sub>H<sub>13</sub>NO<sub>2</sub>

**Molecular Weight:** 143.185

**Accurate Mass:** 143.094629

**Percentage Composition:** C 58.72%; H 9.15%; N 9.78%; O 22.35%

**Physical Description:** Cryst. (petrol)

**Melting Point:** Mp 26-27°

**Boiling Point:** Bp<sub>1</sub> 80°

#### References:

*Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 675A; 675B, (*ir*)

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Con, J.J. *et al.*, *Can. J. Chem.*, 1953, **31**, 1211, (*synth, nitrile*)

Krueger, C., *J. Organomet. Chem.*, 1967, **9**, 125, (*synth, nitrile*)

Kato, T. *et al.*, *Tetrahedron*, 1967, **23**, 2965, (*amide*)

Sánchez, A.G. *et al.*, *J.C.S. Perkin 2*, 1973, 15-20, (*isopropyl ester, synth, pmr, ir*)

Deswarte, S. *et al.*, *Bull. Soc. Chim. Belg.*, 1975, **84**, 321, (*spectra, nitrile*)

Dedina, J. *et al.*, *Coll. Czech. Chem. Comm.*, 1975, **40**, 3476, (*isom, nitrile*)

Kato, T. *et al.*, *Heterocycles*, 1975, **3**, 413, (*amide, rev*)

Buckler, R.T. *et al.*, *J. Med. Chem.*, 1975, **18**, 509

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