



>>Variant: (ξ)-form

Molecular Formula: C₄H₇NO₂

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: C₅H₉NO₂

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: C₆H₁₁NO₂

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: C₇H₁₃NO₂

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: Bp₁ 80°

References:

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

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1072C; 1073A, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 733C; 733D, (*ir*)

Mumm, O. *et al.*, *Ber.*, 1922, **55**, 2068, (*ester*)

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

Hiyama, T. *et al.*, *Tet. Lett.*, 1982, **23**, 1597