



>>Entry Name: Diethylcarbamic acid, 9CI

CAS Registry Number: 24579-70-2
Et₂NCOOH

Molecular Formula: C₅H₁₁NO₂
Molecular Weight: 117.147
Accurate Mass: 117.078979
Percentage Composition: C 51.26%; H 9.46%; N 11.96%; O 27.31%
Other Data: Unstable above -15°

>>Derivative: Me ester

CAS Registry Number: 4652-44-2
Molecular Formula: C₆H₁₃NO₂
Molecular Weight: 131.174
Accurate Mass: 131.094629
Percentage Composition: C 54.94%; H 9.99%; N 10.68%; O 24.39%
Boiling Point: Bp₃₀ 34-36°

>>Derivative: Chloride

Synonym(s): *N*-Diethylchloroformamide. Diethylcarbamoyl chloride

CAS Registry Number: 88-10-8
Molecular Formula: C₅H₁₀ClNO
Molecular Weight: 135.593
Accurate Mass: 135.045091
Percentage Composition: C 44.29%; H 7.43%; Cl 26.15%; N 10.33%; O 11.80%
Boiling Point: Bp 186° (190-195°)

Aldrich: D9140-3
Fluka: 32050

>>Derivative: Nitrile

Synonym(s): Diethylcyanamide

CAS Registry Number: 617-83-4
Molecular Formula: C₅H₁₀N₂
Molecular Weight: 98.147
Accurate Mass: 98.084398
Percentage Composition: C 61.19%; H 10.27%; N 28.54%
Use/Importance: Dehydrating agent for coupling of *N*-protected aminoacids
Boiling Point: Bp 190°. Bp₁₀ 68°

Aldrich: 21381-0

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1217B; 1309B; 1377C, (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 743B; 802C; 856A, (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 791A; 813A, (*ir*)
Wallach, O., *Ber.*, 1899, **32**, 1872, (*synth, nitrile*)
Campbell, A.W. *et al.*, *Ind. Eng. Chem.*, 1953, **45**, 125, (*synth*)
Ried, W. *et al.*, *Annalen*, 1954, **590**, 123, (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 249, (*nitrile*)
Sellakumar, A.R. *et al.*, *J. Environ. Pathol. Toxicol.*, 1980, 107, (*tox, chloride*)
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