



>>Entry Name: Cyanoacetaldehyde

Synonym(s): 3-Oxopropanenitrile, 9Cl. Malonaldehydic nitrile. Formylacetonitrile

CAS Registry Number: 6162-76-1

NCCH₂CHO

Molecular Formula: C₃H₃NO

Molecular Weight: 69.063

Accurate Mass: 69.021464

Percentage Composition: C 52.17%; H 4.38%; N 20.28%; O 23.17%

Physical Description: Liq.

Boiling Point: Bp 71-72°

Solubility: Misc. EtOH, Et₂O, CHCl₃

Density: d¹⁵ 0.88

>>Derivative: 2,4-Dinitrophenylhydrazone

Physical Description: Cryst. (EtOH)

Melting Point: Mp 170-171°

>>Derivative: Di-Me acetal

Synonym(s): 3,3-Dimethoxypropanenitrile, 9Cl. 2-Cyano-1,1-dimethoxyethane

CAS Registry Number: 57597-62-3

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: Oil

Boiling Point: Bp₅ 89°

Aldrich: 36235-2

>>Derivative: Di-Et acetal

Synonym(s): 3,3-Diethoxypropanenitrile. 2-Cyano-1,1-diethoxyethane

CAS Registry Number: 2032-34-0

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%

Boiling Point: Bp₁₄ 99°

Aldrich: 37861-5

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1373B; 1375C, (*nmr*)

Claisen, L., *Ber.*, 1903, **36**, 3665, (*synth*)

Hartung, W.H. *et al.*, *J.A.C.S.*, 1927, **49**, 2520, (*synth*)

Jachak, M. *et al.*, *Synthesis*, 1992, 275, (*synth, acetal, ir, pmr*)