



Molecular Weight: 176.212
Accurate Mass: 176.10486
Percentage Composition: C 54.53%; H 9.15%; O 36.32%
Boiling Point: Bp 199°. Bp₁₃ 83-85°
Aldrich: 12824-4
Fluka: 31638

>>**Derivative:** Di-Et acetal, amide

CAS Registry Number: 61189-99-9
Molecular Formula: C₆H₁₃NO₃
Molecular Weight: 147.174
Accurate Mass: 147.089544
Percentage Composition: C 48.97%; H 8.90%; N 9.52%; O 32.61%
Boiling Point: Subl. 81.5°
Aldrich: 37045-2
Fluka: 31603

>>**Derivative:** Di-Et acetal, nitrile
Synonym(s): Cyanodiethoxymethane

CAS Registry Number: 6136-93-2
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%
Boiling Point: Bp₁₂ 55-56°
Aldrich: 37046-0

>>**Derivative:** Di-Et mercaptal, Et ester
Synonym(s): Ethyl bis(ethylthio)acetate

CAS Registry Number: 20461-95-4
Molecular Formula: C₈H₁₆O₂S₂
Molecular Weight: 208.345
Accurate Mass: 208.05917
Percentage Composition: C 46.12%; H 7.74%; O 15.36%; S 30.78%
Use/Importance: Used for synthesis of 1,4-dicarbonyl compds.
Physical Description: Liq.
Boiling Point: Bp_{0.1} 70°
Refractive Index: n_D²⁰ 1.4970
Aldrich: 22634-3
Fluka: 50708

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 521D; 667B, (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1049B; 1049C; 1225C; 1375B, (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 723D; 724A, (*ir*)
Scheibler, H. *et al.*, *Ber.*, 1934, **67**, 1507, (*amide*)
Eisenbraun, A.A. *et al.*, *Can. J. Chem.*, 1960, **38**, 622, (*synth*)
Org. Synth., Coll. Vol., 4, 1963, 124; 427, (*synth*)
Org. Synth., Coll. Vol., 4, 1963, 124-125, (*butyl ester*)
Blake, J. *et al.*, *J.A.C.S.*, 1966, **88**, 4061, (*tert-butyl ester*)
Pappas, J.J. *et al.*, *Tet. Lett.*, 1966, 4273, (*synth*)
Kelly, T.R. *et al.*, *Synthesis*, 1972, 544, (*synth*)
Ullmanns Encykl. Tech. Chem., 4. Aufl., 1976, 1976, (*rev*)
Brain, E.G. *et al.*, *J.C.S. Perkin 1*, 1977, 2479-2487, (*4-nitrobenzyl ester*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1979, **7**, 162; **9**, 228
Huet, F. *et al.*, *Synthesis*, 1979, 33, (*Di-Me acetal*)
U.S. Pat., 1979, 4 140 676; *CA*, **90**, 188904h, (*polymers*)
Lissel, M. *et al.*, *Annalen*, 1982, 1589, (*di-Et mercaptal, Et ester*)
Ezerskaya, N.A. *et al.*, *Zh. Anal. Khim.*, 1988, **43**, 846, (*synth, detn, Rh*)
Merck Index, 11th edn., 1989, 4407
Bishop, J.E. *et al.*, *J.O.C.*, 1991, **56**, 5079, (*benzyl, tert-butyl esters*)
Seip, J.E. *et al.*, *J.O.C.*, 1993, **58**, 2253, (*manuf*)
O'Brien, P. *et al.*, *J.C.S. Perkin 1*, 1996, 2117, (*Me ester, synth, pmr*)
Brimble, M.A. *et al.*, *Synth. Commun.*, 1996, **26**, 243, (*butyl ester*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, GIQ000; MKI550