



Percentage Composition: C 39.98%; H 6.71%; O 31.96%; S 21.35%

Use/Importance: Reagent for synth. of α,β -unsatd. esters

>> **Derivative:** *S,S*-Dioxide

CAS Registry Number: 2516-97-4

Molecular Formula: $C_3H_6O_4S$

Molecular Weight: 138.144

Accurate Mass: 137.99868

Percentage Composition: C 26.08%; H 4.38%; O 46.33%; S 23.21%

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 114°

Other: Oakwood 3739

>> **Derivative:** *S,S*-Dioxide, Me ester

CAS Registry Number: 62020-09-1

Molecular Formula: $C_4H_8O_4S$

Molecular Weight: 152.171

Accurate Mass: 152.01433

Percentage Composition: C 31.57%; H 5.30%; O 42.06%; S 21.07%

Physical Description: Cryst. (EtOH/2-propanol)

Melting Point: Mp 65.5-66.5°

Other: Oakwood 3762

>> **Derivative:** *S,S*-Dioxide, Et ester

CAS Registry Number: 4455-15-6

Molecular Formula: $C_5H_{10}O_4S$

Molecular Weight: 166.198

Accurate Mass: 166.02998

Percentage Composition: C 36.13%; H 6.06%; O 38.51%; S 19.29%

Boiling Point: $Bp_{0.2}$ 111-113°

Fluka: 69229

Other: Oakwood 3724

>> **Derivative:** *S,S*-Dioxide, nitrile

Synonym(s): (Methylsulfonyl)acetonitrile, 9Cl. Cyano(methylsulfonyl)methane. Cyanomethyl methyl sulfone

CAS Registry Number: 2274-42-2

Molecular Formula: $C_3H_5NO_2S$

Molecular Weight: 119.144

Accurate Mass: 119.004099

Percentage Composition: C 30.24%; H 4.23%; N 11.76%; O 26.86%; S 26.91%

Use/Importance: Dye intermed.

Physical Description: Cryst. (H_2O)

Melting Point: Mp 83.5-84.5°

References:

Aldrich Library of ^{13}C and 1H FT NMR Spectra, 1992, **1**, 819B; 1064A; 1064B; 1372B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 670B; 853B, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 729B; 811A, (*ir*)

Larsson, E., *Ber.*, 1930, **63**, 1347, (*synth*)

Dijkstra, R. *et al.*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1954, **73**, 569, (*deriv, synth, bibl, nitrile*)

Carpenter, J.M. *et al.*, *J.C.S.(C)*, 1970, 2016, (*S,S-dioxide, synth*)

Huppertz, J.L., *Aust. J. Chem.*, 1971, **24**, 653, (*S,S-Dioxide-Et ester*)

Hsi, K.L. *et al.*, *Sci. Sin. (Engl. edn.)*, 1974, **17**, 743, (*deriv, synth*)

v. Asten, J.J.A. *et al.*, *Tet. Lett.*, 1975, 671, (*Ethyl α -methylsulfinylacetate*)

U.S. Pat., 1976, 3 931 358; *CA*, **84**, 150388, (*synth, nitrile*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1977, **6**, 255, (*Ethyl α -methylsulfinylacetate*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 349

Gipstein, E. *et al.*, *J.O.C.*, 1980, **45**, 1486, (*S,S-dioxide Me ester, synth, pmr*)

Mathias, E. *et al.*, *Chem. Comm.*, 1981, 569, (*synth, ir, pmr, cmr, haz*)

Takagi, T., *Bull. Chem. Soc. Jpn.*, 1984, **57**, 1299, (*cmr*)

Kimura, M. *et al.*, *Chem. Comm.*, 1987, 122, (*dioxide, synth*)