



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. (H₂O)

Melting Point: Mp 83.5-84.5°

References:

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

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