



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

CAS Registry Number: 6274-54-0

Molecular Formula: C₁₀H₁₂O₄S

Molecular Weight: 228.268

Accurate Mass: 228.04563

Percentage Composition: C 52.62%; H 5.30%; O 28.04%; S 14.05%

Melting Point: Mp 95-96°

>>Derivative: S,S-Dioxide, chloride

CAS Registry Number: 40913-92-6

Molecular Formula: C₈H₇ClO₃S

Molecular Weight: 218.66

Accurate Mass: 217.980442

Percentage Composition: C 43.94%; H 3.23%; Cl 16.21%; O 21.95%; S 14.66%

Melting Point: Mp 132°

>>Derivative: S,S-Dioxide, amide

Molecular Formula: C₈H₉NO₃S

Molecular Weight: 199.23

Accurate Mass: 199.030314

Percentage Composition: C 48.23%; H 4.55%; N 7.03%; O 24.09%; S 16.09%

Melting Point: Mp 248-250 dec.°

>>Derivative: S,S-Dioxide, nitrile

CAS Registry Number: 22821-76-7

Molecular Formula: C₈H₇NO₂S

Molecular Weight: 181.215

Accurate Mass: 181.019749

Percentage Composition: C 53.02%; H 3.89%; N 7.73%; O 17.66%; S 17.70%

Physical Description: Cryst. (Me₂CO aq.)

Melting Point: Mp 142° (134-135°)

References:

- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **2**, 1084B; 1586B, (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 196C; 487C, (*ir*)
Buu-Hoï, N.P., *Bull. Soc. Chim. Fr.*, 1946, 139, (*synth, derivs*)
Price, C.C. *et al.*, *J.A.C.S.*, 1952, **74**, 1943, (*synth, uv, dioxide*)
Baker, J.W. *et al.*, *J.C.S.*, 1952, 2831, (*synth*)
Szmant, H.H. *et al.*, *J.A.C.S.*, 1956, **78**, 3400, (*synth*)
Kidd, D.A.A. *et al.*, *J.C.S.*, 1962, 1420, (*dioxide, nitrile*)
Baarschers, W.H. *et al.*, *Can. J. Chem.*, 1973, **51**, 156, (*ms, dioxide*)
Beckwith, A.L.J. *et al.*, *Aust. J. Chem.*, 1986, **39**, 77, (*nitrile, synth, pmr*)
Brown, R.W. *et al.*, *J.O.C.*, 1991, **56**, 4974, (*synth, dioxide*)
Pizzo, F. *et al.*, *Synth. Commun.*, 1994, **24**, 2665, (*dioxide*)