



>>Entry Name: Ethoxycarbonyl isothiocyanate

Synonym(s): Ethyl carbon(isothiocyanatidate),9Cl. Carbonic acid monoanhydride with isothiocyanic acid ethyl ester, 8Cl. Carbethoxyl isothiocyanate. Carbethoxythiocarbimide. Ethyl thiocyanofomate

CAS Registry Number: 16182-04-0
EtOOCNCS

Molecular Formula: C₄H₅NO₂S

Molecular Weight: 131.155

Accurate Mass: 131.004099

Percentage Composition: C 36.63%; H 3.84%; N 10.68%; O 24.40%; S 24.45%

Use/Importance: Reagent for synth. of heterocyclic compds.

Physical Description: Oil

Boiling Point: Bp₁₀ 44-46°. Bp_{0.6} 37-38°

Refractive Index: n_D²³ 1.4960

Hazard & Toxicity: Eye and respiratory tract irritant

Aldrich: 19612-6

Fluka: 2590

References:

- Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 873B, (*ir*)
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Takamizawa, A. *et al.*, *Bull. Chem. Soc. Jpn.*, 1963, **36**, 1214-1220, (*synth, ir, uv, use*)
Lamon, R.W., *J. Het. Chem.*, 1968, **5**, 837-844, (*synth, use*)
Goerdeler, J. *et al.*, *Chem. Ber.*, 1971, **104**, 1606-1610, (*synth, use*)
Liotta, D. *et al.*, *Can. J. Chem.*, 1975, **53**, 907-912, (*synth, use, ir, pmr, ms*)
Esmail, R. *et al.*, *Synthesis*, 1975, 301-314, (*rev*)
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George, B. *et al.*, *J. Het. Chem.*, 1983, **20**, 1127-1142, (*rev*)
Katritzky, A.R. *et al.*, *Org. Prep. Proced. Int.*, 1993, **25**, 83-90, (*use, bibl*)