



>>Entry Name: Cyanocarbamodithioic acid, 9CI

Synonym(s): Cyanocarbonimidodithioic acid. Cyanodithioimidocarbonic acid. Cyanimidodithiocarbonic acid

CAS Registry Number: 108-04-3

Related CAS Registry Numbers(s): 34318-05-3 35092-86-5

$(\text{HS})_2\text{C}=\text{NCN} \leftrightarrow \text{HSC}(\text{S})\text{NHCN}$

Molecular Formula: $\text{C}_2\text{H}_2\text{N}_2\text{S}_2$

Molecular Weight: 118.183

Accurate Mass: 117.965938

Percentage Composition: C 20.33%; H 1.71%; N 23.70%; S 54.26%

General Statement: Existence of free acid doubtful

>>Derivative: Di-K salt

CAS Registry Number: 13145-41-0

Use/Importance: Reagent for synth. of heterocycles

Melting Point: Mp 217-225°

>>Derivative: Di-Me ester

Synonym(s): Dimethyl cyanodithioiminocarbonate. DMT

CAS Registry Number: 10191-60-3

Molecular Formula: $\text{C}_4\text{H}_6\text{N}_2\text{S}_2$

Molecular Weight: 146.237

Accurate Mass: 145.997238

Percentage Composition: C 32.85%; H 4.14%; N 19.16%; S 43.85%

Use/Importance: Intermed. for heterocyclic synth., available industrially

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 51-52.5°

Aldrich: 24963-7

References:

- Aldrich Library of FT-IR Spectra*, 1st edn., 1985, **1**, 867A, (ir)
Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1394C, (nmr)
Hantzsch, A. *et al.*, *Annalen*, 1904, **331**, 265, (synth)
Timmons, R.J. *et al.*, *J.O.C.*, 1967, **32**, 1566, (synth, use)
Jensen, K.A. *et al.*, *Acta Chem. Scand.*, 1968, **22**, 1107, (synth, use)
Thalev, W.A. *et al.*, *J.O.C.*, 1971, **36**, 14, (synth, K salt)
Wobig, D. *et al.*, *Annalen*, 1972, **764**, 125, (synth, use)
Wittenbrook, L.S. *et al.*, *J.O.C.*, 1973, **38**, 465, (synth, use)
Gattow, G. *et al.*, *Z. Anorg. Allg. Chem.*, 1977, **433**, 211; **434**, 115, (synth, ir)
Klasinc, L. *et al.*, *Gazz. Chim. Ital.*, 1980, **110**, 287, (di-Me ester, pmr, uv)
Yokoyama, M. *et al.*, *J.C.S. Perkin I*, 1988, 2309, (di-Me ester, ir, pmr)
Tominaga, Y. *et al.*, *J. Het. Chem.*, 1991, **28**, 1039, (di-Me ester, use, bibl)
Marble, L.K., *Org. Prep. Proced. Int.*, 1998, **30**, 473-476, (di-Me ester, synth, pmr, cmr)