



>>Entry Name: 2-Cyanoethanethioamide, 9CI

Synonym(s): 2-Cyanothioacetamide, 8CI

CAS Registry Number: 7357-70-2

NCCH₂CSNH₂

Molecular Formula: C₃H₄N₂S

Molecular Weight: 100.144

Accurate Mass: 100.009518

Percentage Composition: C 35.98%; H 4.03%; N 27.97%; S 32.02%

Use/Importance: Reactive compd. for the synth. of *N*- and *S*-heterocycles

Physical Description: Cryst. (EtOH or C₆H₆)

Melting Point: Mp 121-123°

Other Data: Darkens on long standing

Aldrich: 27246-9

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1335B, (*nmr*)

Riad, B.Y. *et al.*, *Heterocycles*, 1987, **26**, 205, (*rev*)

Elgemeie, G.E.H. *et al.*, *Bull. Chem. Soc. Jpn.*, 1993, **66**, 555, (*use*)