



>>Entry Name: 1-Isothiocyanto-3-nitrobenzene, 9CI

Synonym(s): 3-Nitrophenyl isothiocyanate

CAS Registry Number: 3529-82-6

Molecular Formula: $C_7H_4N_2O_2S$

Molecular Weight: 180.187

Accurate Mass: 179.999348

Percentage Composition: C 46.66%; H 2.24%; N 15.55%; O 17.76%; S 17.80%

Physical Description: Needles (AcOH)

Melting Point: Mp 60.5°

Boiling Point: Bp 275-280° dec.

Solubility: Spar. sol. H_2O

References:

Steudemann, H., *Ber.*, 1883, **16**, 549; 2334

Danihel, I. *et al.*, *Chem. Zvesti*, 1984, **38**, 539, (*cmr*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, ISO000