



>>Entry Name: 1-Isothiocyanato-4-nitrobenzene, 9CI

Synonym(s): 4-Nitrophenyl isothiocyanate

CAS Registry Number: 2131-61-5

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: Pale-yellow needles (AcOH)

Melting Point: Mp 112-113°

Aldrich: 28354-1

Fluka: 73728

References:

Aldrich Library of ^{13}C and 1H FT NMR Spectra, 1992, **2**, 1559B, (*nmr*)

Jacobson, P. *et al.*, *Ber.*, 1893, **26**, 2369