



>>Entry Name: (4-Nitrophenyl)thiourea, 9CI

Synonym(s): 1-(*p*-Nitrophenyl)-2-thiourea, 8CI

CAS Registry Number: 3696-22-8

Molecular Formula: C₇H₇N₃O₂S

Molecular Weight: 197.217

Accurate Mass: 197.025897

Percentage Composition: C 42.63%; H 3.58%; N 21.31%; O 16.23%; S 16.26%

Use/Importance: Active against tuberculosis in mice

Physical Description: Yellow cryst.

Melting Point: Mp 189-190°. Mp 206°

pKa Value: p*K*_a 10.75 (25°, H₂O) p*K*_a 15.05 (25°, MeOH)

Aldrich: 19937-0

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 417D, (*ir*)

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 387C, (*nmr*)

Dyson, G.M. *et al.*, *J.C.S.*, 1924, **125**, 1707, (*synth*)

Neville, R.G. *et al.*, *Can. J. Chem.*, 1963, **41**, 2123, (*synth*)

Kavalek, J. *et al.*, *Coll. Czech. Chem. Comm.*, 1983, **48**, 1430, (*pka*)