



>>Entry Name: Methylthiourea, 9CI

CAS Registry Number: 598-52-7

MeNHCSNH₂

Molecular Formula: C₂H₆N₂S

Molecular Weight: 90.149

Accurate Mass: 90.025168

Percentage Composition: C 26.65%; H 6.71%; N 31.07%; S 35.57%

Physical Description: Prisms (EtOH)

Melting Point: Mp 120.5-121°

Solubility: Sol. H₂O

pKa Value: pK_a 9.81 (25°)

Hazard & Toxicity: Exp. teratogen

Aldrich: M8460-7

Fluka: 69350

Sigma: M0520

>>Derivative: N'-Benzyl

Synonym(s): N-Benzyl-N'-methylthiourea

CAS Registry Number: 2740-94-5

Molecular Formula: C₉H₁₂N₂S

Molecular Weight: 180.273

Accurate Mass: 180.072118

Percentage Composition: C 59.96%; H 6.71%; N 15.54%; S 17.79%

Melting Point: Mp 74-76°

Aldrich: 27550-6

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1336A, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 827C, (*ir*)

Org. Synth., 1941, **21**, 83, (*synth*)

Nair, G.V. *et al.*, *Indian J. Chem.*, 1966, **4**, 516, (*synth*)

Singh, H. *et al.*, *Chem. Ind. (London)*, 1977, 984, (*synth*)

Filleux-Blanchard, M.L., *Org. Magn. Reson.*, 1977, **9**, 125, (*cmr, conformn*)

Singh, H. *et al.*, *J.C.S. Perkin I*, 1980, 1013, (*synth*)

Sullivan, R.H. *et al.*, *Org. Magn. Reson.*, 1983, **21**, 293, (*cmr, conformn*)

Schelenz, T. *et al.*, *Biochem. Physiol. Pflanz.*, 1986, **181**, 359, (*synth*)

Mido, Y. *et al.*, *Spectrochim. Acta A*, 1988, **44**, 661, (*ir, Raman*)

Sibi, M.P., *Magn. Reson. Chem.*, 1991, **29**, 401, (*N-15 nmr*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, MPW600