



>>Entry Name: Benzyl carbamimidothioate

Synonym(s): Phenylmethyl carbamimidothioate, 9Cl. 2-Benzyl-2-thiopseudourea, 8Cl

CAS Registry Number: 621-85-2

PhCH2SC(NH2)=NH

Molecular Formula: C₈H₁₀N₂S

Molecular Weight: 166.246

Accurate Mass: 166.056468

Percentage Composition: C 57.80%; H 6.06%; N 16.85%; S 19.29%

>>Derivative: Hydrochloride

Synonym(s): S-Benzylthiuronium chloride

CAS Registry Number: 538-28-3

Molecular Formula: C₈H₁₁ClN₂S

Molecular Weight: 202.707

Accurate Mass: 202.033145

Percentage Composition: C 47.40%; H 5.47%; Cl 17.49%; N 13.82%; S 15.82%

Use/Importance: Reference material used in elemental microanalysis. Reagent for the isolation and identification of org. acids

Physical Description: Cryst.

Melting Point: Mp 146-148°. Mp 172-174° (dimorph.)

Aldrich: 25103-8

Fluka: 13520

Rare Chemicals Library: S37647-7

Sigma: B9138

>>Derivative: Hydrobromide

CAS Registry Number: 55796-74-2

Physical Description: Cryst. (EtOH)

Melting Point: Mp 127-128°

>>Derivative: Hydroiodide

CAS Registry Number: 55796-75-3

Physical Description: Cryst. (EtOH)

Melting Point: Mp 140°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, 2, 416A, (ir)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, 2, 1473B, (nmr)

Donleavy, J.J., *J.A.C.S.*, 1936, **58**, 1004, (*synth, use*)

Friediger, A. *et al.*, *Acta Chem. Scand.*, 1955, **9**, 1425, (*use*)

Bharagava, P.N. *et al.*, *J. Indian Chem. Soc.*, 1955, **32**, 283-284, (*hydrobromide, hydroiodide, synth*)

Analyst (London), 1972, **97**, 740, (*microanal*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BEU500