



>>Entry Name: Benzoyl isothiocyanate, 9CI

Synonym(s): Benzoic acid anhydride with isothiocyanic acid, 8CI

CAS Registry Number: 532-55-8

PhCONCS

Molecular Formula: C₈H₅NOS

Molecular Weight: 163.2

Accurate Mass: 163.009184

Percentage Composition: C 58.88%; H 3.09%; N 8.58%; O 9.80%; S 19.65%

Physical Description: Oil

Boiling Point: Bp₁₈ 133-137°

Density: d¹⁸ 1.214

Aldrich: 26165-3

Fluka: 13007

Rare Chemicals Library: S54765-4

Sigma: B9134

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1561A, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 465B, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1426B, (*ir*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 50

Kristian, P. *et al.*, *Coll. Czech. Chem. Comm.*, 1977, **42**, 671, (*ir, struct*)

Heinz, P. *et al.*, *Monatsh. Chem.*, 1977, **108**, 665, (*synth*)

Kniesz, L. *et al.*, *Synth. Commun.*, 1990, **20**, 509, (*synth*)