



>>Entry Name: Benzenesulfonyl isocyanate, 9CI

CAS Registry Number: 2845-62-7

PhSO₂NCO

Molecular Formula: C₇H₅NO₃S

Molecular Weight: 183.187

Accurate Mass: 182.999014

Percentage Composition: C 45.90%; H 2.75%; N 7.65%; O 26.20%; S 17.50%

Use/Importance: Used for characterisation of hindered alcohols and phenols

Physical Description: Liq.

Boiling Point: Bp₉ 129°. Bp₃ 90°

Aldrich: 23229-7

Fluka: 12701

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1647B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 487B, (*ir*)

Franz, J.E. *et al.*, *J.O.C.*, 1964, **29**, 2592, (*synth*)

McFarland, J.W. *et al.*, *J.O.C.*, 1965, **30**, 957, (*synth*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 48

Appel, R. *et al.*, *Chem. Ber.*, 1974, **107**, 706, (*synth*)