



>>Entry Name: Benzoyl isocyanate, 9CI

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

CAS Registry Number: 4461-33-0

PhCON=C=O

Molecular Formula: C₈H₅NO₂

Molecular Weight: 147.133

Accurate Mass: 147.032029

Percentage Composition: C 65.31%; H 3.43%; N 9.52%; O 21.75%

Physical Description: Prisms (Et₂O)

Melting Point: Mp 26°

Boiling Point: Bp₇₂₄ 202°. Bp₂₀ 88-91°

Other Data: Polymerises on storage

Aldrich: 30818-8

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1563C, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1427D, (*ir*)

Billeter, O.C., *Ber.*, 1903, **36**, 3218, (*synth*)

Hill, A.J. *et al.*, *J.A.C.S.*, 1940, **62**, 1595, (*synth*)