



>>Entry Name: Benzyl bromide

Synonym(s): (Bromomethyl)benzene, 9CI. α -Bromotoluene, 8CI

CAS Registry Number: 100-39-0

PhCH₂Br

Molecular Formula: C₇H₇Br

Molecular Weight: 171.036

Accurate Mass: 169.993111

Percentage Composition: C 49.16%; H 4.13%; Br 46.72%

Use/Importance: Benzylating agent showing selectivity. Reagent for anal. of ethylenethiourea

Physical Description: Liq.

Melting Point: Mp -4°

Boiling Point: Bp 198°. Bp₈₀ 127°

Density: d₀²²1.438

Hazard & Toxicity: Fl. p. 87°. Storage over molecular sieve causes build-up of HBr. Irritating and corrosive to all tissues. Lachrymator

Aldrich: B1790-5

Fluka: 13250

Sigma: B1012

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 63B, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 973A, (ir)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 890B, (ir)

Schramm, J., *Ber.*, 1885, **18**, 606, (synth)

Newsome, W.H., *J. Agric. Food Chem.*, 1972, **20**, 967, (use)

Olah, G.A. *et al.*, *Synthesis*, 1974, 653, (synth)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 25

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, BEC000

Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th edn., Butterworths, 1990, 2565

Luxon, S.G., *Hazards in the Chemical Laboratory*, 5th edn., Royal Society of Chemistry, 1992, 123