



>>Entry Name: Benzyl chloride

Synonym(s): (Chloromethyl)benzene, 9Cl. α -Chlorotoluene, 8Cl

CAS Registry Number: 100-44-7

Related CAS Registry Numbers(s): 59502-05-5

PhCH₂Cl

Molecular Formula: C₇H₇Cl

Molecular Weight: 126.585

Accurate Mass: 126.023627

Percentage Composition: C 66.42%; H 5.57%; Cl 28.01%

Source/Synthesis: Produced by thermal or photochemical chlorination of toluene

Use/Importance: Used in manuf. of vinyl resin plasticizers

Physical Description: Liq. with pungent odour

Melting Point: Mp -48°. Mp -43°

Boiling Point: Bp 179°. Bp₆₂ 99°

Density: d₄⁴ 1.11

Other Data: Steam-volatile

Hazard & Toxicity: Can undergo violent metal-catalysed polymerisation if not stabilised. Severe skin, eye and mucous membrane irritant. Lachrymator. Contact with liquid can cause corneal injury and dermatitis. LD₅₀ (rat, orl) 1231 mg/kg; LC₅₀ (rat, ihl) 150 ppm (2 h exposure). Exp. reprod. effects

Aldrich: 32016-1

Fluka: 13280

Sigma: B0887

Supelco: R30-0550

References:

- Aldrich Library of FT-IR Spectra*, 1st edn., 1985, **1**, 972D, (ir)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 63A, (nmr)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 890A, (ir)
Ger. Pat., 1923, 478 084; *CA*, **23**, 4228, (synth)
Kharasch, M.S. *et al.*, *J.A.C.S.*, 1939, **61**, 2142, (synth)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 1080; **3**, 19; **8**, 110; **2**, 158; **4**, 310, (use)
Reynolds, W.F. *et al.*, *Can. J. Chem.*, 1973, **51**, 1857, (cmr)
Nash, R.G., *J. Assoc. Off. Anal. Chem.*, 1974, **57**, 1015, (use)
Bastaert, G. *et al.*, *C. R. Hebd. Seances Acad. Sci. Ser. C*, 1980, **290**, 193, (uv)
Ullmann's Encycl. Ind. Chem., 5th. edn., VCH, Weinheim, 1985, **A6**, 355, (rev)
Schaefer, T. *et al.*, *Can. J. Chem.*, 1986, **64**, 1372, (pmr, conformn)
Morita, M. *et al.*, *J. Appl. Electrochem.*, 1988, **18**, 491, (synth)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **6**, 113, (rev)
Vogel, A.I., *Practical Organic Chemistry*, 5th edn., Longman Scientific and Technical, 864, (synth)
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. *et al.*), J.B. Lippincott, 1988, 109
Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th edn., Butterworths, 1990, 2567
Luxon, S.G., *Hazards in the Chemical Laboratory*, 5th edn., Royal Society of Chemistry, 1992, 125
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, BEE375