



>>Entry Name: 4-(Chloromethyl)phenol

Synonym(s): α -Chloro-*p*-cresol, 8Cl. 4-Hydroxybenzyl chloride

CAS Registry Number: 35421-08-0

Molecular Formula: C₇H₇ClO

Molecular Weight: 142.584

Accurate Mass: 142.018542

Percentage Composition: C 58.97%; H 4.95%; Cl 24.86%; O 11.22%

>>Derivative: Ac

CAS Registry Number: 39720-27-9

Molecular Formula: C₉H₉ClO₂

Molecular Weight: 184.622

Accurate Mass: 184.029107

Percentage Composition: C 58.55%; H 4.91%; Cl 19.20%; O 17.33%

Use/Importance: Reagent for protection of thiols as base-labile 4-acetoxybenzyl sulfides, and of other functional groups

Physical Description: Liq.

Boiling Point: Bp_{1.5} 104-106°. Bp_{0.01} 59-60°

Refractive Index: n_D²⁵ 1.5290

Hazard & Toxicity: Exothermic synthesis

Aldrich: 43288-1

>>Derivative: Me ether

Synonym(s): 1-(Chloromethyl)-4-methoxybenzene. 4-(Chloromethyl)anisole. 4-Methoxybenzyl chloride

CAS Registry Number: 824-94-2

Molecular Formula: C₈H₉ClO

Molecular Weight: 156.611

Accurate Mass: 156.034192

Percentage Composition: C 61.35%; H 5.79%; Cl 22.64%; O 10.22%

Use/Importance: Reagent for *S*-protection in peptide synth.

Boiling Point: Bp₁₉ 113°. Bp_{0.01} 59-60° (64-65°)

Refractive Index: n_D¹⁹ 1.5492

Hazard & Toxicity: Has exploded on storage at r.t.

Aldrich: 27024-5

Fluka: 64870

>>Derivative: Benzyl ether

Synonym(s): 1-(Chloromethyl)-4-(phenylmethoxy)benzene, 9Cl. Benzyl α -chloro-*p*-tolyl ether, 8Cl. 4-Benzyloxybenzyl chloride. 4-(Chloromethyl)- α -phenylanisole

CAS Registry Number: 836-42-0

Molecular Formula: C₁₄H₁₃ClO

Molecular Weight: 232.709

Accurate Mass: 232.065492

Percentage Composition: C 72.26%; H 5.63%; Cl 15.23%; O 6.88%

Use/Importance: Used in manuf. of pharmaceuticals, pesticides and other agrochemicals

Physical Description: Plates (petrol or hexane)

Melting Point: Mp 80-82° (77-79°)

Hazard & Toxicity: Lachrymator

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 188C, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 973D, (*ir*)

Shelton, R.S. *et al.*, *J.A.C.S.*, 1953, **75**, 5491-5495, (*benzyl ether*)

Tait, J.M.S. *et al.*, *J.A.C.S.*, 1962, **84**, 4, (*ms, deriv*)

Grice, R. *et al.*, *J.C.S.*, 1963, 1947, (*synth, deriv*)

Dhami, K.S. *et al.*, *Can. J. Chem.*, 1966, **44**, 2855, (*cmr, deriv*)

Taylor, L.D. *et al.*, *J.O.C.*, 1978, **43**, 1197, (*deriv*)

Alvarez-Ibarra, C. *et al.*, *Tetrahedron*, 1979, **35**, 1767, (*synth, ir, pmr, deriv*)

Battersby, A.R. *et al.*, *J.C.S. Perkin I*, 1980, 31, (*synth, pmr, uv, ms, benzyl ether*)

Amin, S. *et al.*, *J.O.C.*, 1981, **46**, 2394, (*deriv, pmr*)

Aizpurva, J.M. *et al.*, *Can. J. Chem.*, 1986, **64**, 2342, (*deriv*)

Christensen, J.B., *Org. Prep. Proced. Int.*, 1994, **26**, 471, (*synth, Ac*)