



**>>Entry Name: 3-(Chloromethyl)phenol**

**Synonym(s):**  $\alpha$ -Chloro-*m*-cresol, 8Cl. 3-Hydroxybenzyl chloride

**CAS Registry Number:** 60760-06-7

**Molecular Formula:** C<sub>7</sub>H<sub>7</sub>ClO

**Molecular Weight:** 142.584

**Accurate Mass:** 142.018542

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

**Boiling Point:** Bp<sub>0.1</sub> 105-110°

**>>Derivative: Ac**

**CAS Registry Number:** 4530-44-3

**Molecular Formula:** C<sub>9</sub>H<sub>9</sub>ClO<sub>2</sub>

**Molecular Weight:** 184.622

**Accurate Mass:** 184.029107

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

**Boiling Point:** Bp<sub>0.001</sub> 95-98°

**Refractive Index:** n<sub>D</sub><sup>19</sup> 1.5272

**>>Derivative: Me ether**

**Synonym(s):** 1-(Chloromethyl)-3-methoxybenzene. 3-Methoxybenzyl chloride

**CAS Registry Number:** 824-98-6

**Molecular Formula:** C<sub>8</sub>H<sub>9</sub>ClO

**Molecular Weight:** 156.611

**Accurate Mass:** 156.034192

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

**Boiling Point:** Bp<sub>16</sub> 102-104°. Bp<sub>0.1</sub> 58°

**Refractive Index:** n<sub>D</sub><sup>20</sup> 1.5427

**Aldrich:** 20938-4

**Fluka:** 64868

**>>Derivative: Ph ether**

**Synonym(s):** 1-(Chloromethyl)-3-phenoxybenzene, 9Cl. 3-Phenoxybenzyl chloride

**CAS Registry Number:** 53874-66-1

**Molecular Formula:** C<sub>13</sub>H<sub>11</sub>ClO

**Molecular Weight:** 218.682

**Accurate Mass:** 218.049842

**Percentage Composition:** C 71.40%; H 5.07%; Cl 16.21%; O 7.32%

**Use/Importance:** Widely used alkylation agent in manuf. of agrochemicals, pesticides, fungicides and other pharmaceuticals

**Boiling Point:** Bp<sub>5</sub> 141-142°

**Refractive Index:** n<sub>D</sub><sup>20</sup> 1.5930

**Hazard & Toxicity:** Corrosive; lachrymator

**References:**

*Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 1041D, (*ir*)

*Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **2**, 183B, (*nmr*)

*Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 969D, (*ir*)

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

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

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

Reimann, E. *et al.*, *Arch. Pharm. (Weinheim, Ger.)*, 1985, **318**, 1105, (*synth, deriv*)

Aizpura, J.M. *et al.*, *Can. J. Chem.*, 1986, **64**, 2342, (*synth, pmr*)

*Eur. Pat.*, 1996, 707 007; *CA*, **125**, 58325a, (*Ph ether*)