



>>Entry Name: 4-(Chloromethyl)benzoic acid, 9Cl

Synonym(s): α -Chloro-*p*-toluic acid. *p*-Carboxybenzyl chloride

CAS Registry Number: 1642-81-5

Molecular Formula: C₈H₇ClO₂

Molecular Weight: 170.595

Accurate Mass: 170.013457

Percentage Composition: C 56.33%; H 4.14%; Cl 20.78%; O 18.76%

Physical Description: Cryst. (EtOH aq. or C₆H₆)

Melting Point: Mp 205° (199-201°)

Aldrich: 27079-2

Fluka: 26559

Sigma: C2797

>>Derivative: Me ester

CAS Registry Number: 34040-64-7

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%

Melting Point: Mp 39-40°

Boiling Point: Bp₃₀ 160-165°

>>Derivative: Chloride

CAS Registry Number: 876-08-4

Molecular Formula: C₈H₆Cl₂O

Molecular Weight: 189.04

Accurate Mass: 187.979569

Percentage Composition: C 50.83%; H 3.20%; Cl 37.51%; O 8.46%

Melting Point: Mp 30-31°. Mp 33-35°

Boiling Point: Bp₂₂ 150-155°

Aldrich: 27078-4

>>Derivative: Amide

CAS Registry Number: 84545-14-2

Molecular Formula: C₈H₈ClNO

Molecular Weight: 169.61

Accurate Mass: 169.029441

Percentage Composition: C 56.65%; H 4.75%; Cl 20.90%; N 8.26%; O 9.43%

Melting Point: Mp 173°

>>Derivative: Nitrile

Synonym(s): 4-(Chloromethyl)benzonitrile, 9Cl. α -Chloro-*p*-tolunitrile. *p*-Cyanobenzyl chloride

CAS Registry Number: 874-86-2

Molecular Formula: C₈H₆ClN

Molecular Weight: 151.595

Accurate Mass: 151.018876

Percentage Composition: C 63.38%; H 3.99%; Cl 23.39%; N 9.24%

Physical Description: Prisms (EtOH or petrol)

Melting Point: Mp 77-78°. Mp 81°

Boiling Point: Bp 263°

Rare Chemicals Library: S26478-4

References:

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **2**, 1078A; 1344C, (*nmr*)

Emerson, W.S. *et al.*, *J.A.C.S.*, 1950, **72**, 5152-5154, (*synth, derivs*)

Baker, J.W. *et al.*, *J.C.S.*, 1956, 404-414, (*nitrile*)

Zamorsky, Z., *Chem. Listy*, 1958, **52**, 1192-1193; *CA*, **52**, 17165, (*synth*)

Exner, O. *et al.*, *Coll. Czech. Chem. Comm.*, 1962, **27**, 2296-2306; 1971, **36**, 534-543, (*ir*)