



>>Entry Name: 3-(Chloromethyl)benzoic acid, 9CI

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

CAS Registry Number: 31719-77-4

Molecular Formula: $C_8H_7ClO_2$

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. (H_2O)

Melting Point: Mp 136-138°

Aldrich: 42431-5

Fluka: 26557

>>Derivative: Me ester

CAS Registry Number: 34040-63-6

Molecular Formula: $C_9H_9ClO_2$

Molecular Weight: 184.622

Accurate Mass: 184.029107

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

Physical Description: Liq.

Boiling Point: Bp_{0.7} 68°

Refractive Index: n_D²¹ 1.5401

>>Derivative: Et ester

CAS Registry Number: 54589-54-7

Molecular Formula: $C_{10}H_{11}ClO_2$

Molecular Weight: 198.648

Accurate Mass: 198.044757

Percentage Composition: C 60.46%; H 5.58%; Cl 17.85%; O 16.11%

Boiling Point: Bp₂₅ 168-169°

>>Derivative: Chloride

CAS Registry Number: 63024-77-1

Molecular Formula: $C_8H_6Cl_2O$

Molecular Weight: 189.04

Accurate Mass: 187.979569

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

Boiling Point: Bp₂₀ 149-150°

Aldrich: 26366-4

>>Derivative: Amide

CAS Registry Number: 135654-16-9

Molecular Formula: C_8H_8ClNO

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 124°

>>Derivative: Nitrile

Synonym(s): 3-(Chloromethyl)benzonitrile, 9CI. α -Chloro-*m*-tolunitrile

CAS Registry Number: 64407-07-4

Molecular Formula: C_8H_6ClN

Molecular Weight: 151.595

Accurate Mass: 151.018876

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

Physical Description: Cryst. (EtOH)

Melting Point: Mp 67°

Boiling Point: Bp 258-260°

References: