



>>Entry Name: *N*-Methylphenylcarbamic acid, 9Cl

Synonym(s): *N*-Methylcarbanilic acid, 8Cl

PhNMeCOOH

Molecular Formula: C₈H₉NO₂

Molecular Weight: 151.165

Accurate Mass: 151.063329

Percentage Composition: C 63.57%; H 6.00%; N 9.27%; O 21.17%

>>Derivative: Me ester

CAS Registry Number: 28685-60-1

Molecular Formula: C₉H₁₁NO₂

Molecular Weight: 165.191

Accurate Mass: 165.078979

Percentage Composition: C 65.44%; H 6.71%; N 8.48%; O 19.37%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 44°

Solubility: Sol. Et₂O, petrol, hot conc. HCl

>>Derivative: Et ester

Synonym(s): Methylphenylurethane

CAS Registry Number: 2621-79-6

Molecular Formula: C₁₀H₁₃NO₂

Molecular Weight: 179.218

Accurate Mass: 179.094629

Percentage Composition: C 67.02%; H 7.31%; N 7.82%; O 17.85%

Boiling Point: Bp 243-244°. Bp₁₈ 127-128°

Aldrich: 30951-6

Rare Chemicals Library: S35339-6

>>Derivative: 3-Nitrophenyl ester

Physical Description: Cryst. (EtOH)

Melting Point: Mp 105°

>>Derivative: Chloride

CAS Registry Number: 4285-42-1

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%

Use/Importance: Acylating reagent for aromatic compds.

Physical Description: Plates (EtOH)

Melting Point: Mp 88-89°

Boiling Point: Bp 280°

Aldrich: 32876-6

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1358A; 1425C, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1396C, (*ir*)

Boehm, T. *et al.*, *Ber.*, 1938, **71**, 1797

Dannley, R.L. *et al.*, *J.O.C.*, 1955, **20**, 92

Leister, N.A. *et al.*, *J.O.C.*, 1958, **23**, 1152

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 694