



>>Entry Name: 3-Aminobenzoic acid, 9CI

CAS Registry Number: 99-05-8

Extra CAS Registry Numbers(s): 1321-11-5

Molecular Formula: $C_7H_7NO_2$

Molecular Weight: 137.138

Accurate Mass: 137.047679

Percentage Composition: C 61.31%; H 5.14%; N 10.21%; O 23.33%

Use/Importance: Used as 2% aq. soln. (neutralised with Na_2CO_3) in photometric detn. of Os. Monomer for polyamide fibres

Physical Description: Needles (H_2O)

Melting Point: Mp 178°

Solubility: Sol. alkalis, acids; spar. sol. H_2O , EtOH, Et_2O

pKa Value: pK_{a1} 3.07; pK_{a2} 4.79 (25°,acid)

Aldrich: 12767-1

Fluka: 6920

Sigma: A5393

>>Derivative: Hydrochloride

CAS Registry Number: 15151-51-6

Physical Description: Needles (H_2O)

Melting Point: Mp 286 dec.°

Aldrich: 28965-5

Fluka: 6980

>>Derivative: Me ester

CAS Registry Number: 4518-10-9

Molecular Formula: $C_8H_9NO_2$

Molecular Weight: 151.165

Accurate Mass: 151.063329

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

Physical Description: Leaflets (Et_2O)

Melting Point: Mp 54°

Boiling Point: Bp_1 126°

pKa Value: pK_{a1} 3.58 (25°, 1% EtOH)

Rare Chemicals Library: S66222-4

>>Derivative: Et ester

CAS Registry Number: 582-33-2

Molecular Formula: $C_9H_{11}NO_2$

Molecular Weight: 165.191

Accurate Mass: 165.078979

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

Physical Description: Oil

Boiling Point: Bp 294°. Bp_5 144°

Aldrich: E1050-5

>>Derivative: Et ester, methanesulfonate salt (1:1)

Synonym(s): Tricaine. Metacain. Finquel. MS 222. TS 222

CAS Registry Number: 886-86-2

Use/Importance: Anaesthetic for fish

Physical Description: Cryst. (EtOH/EtOAc)

Melting Point: Mp 149-150°