



>>Entry Name: 3-Amino-4-hydroxybenzoic acid

CAS Registry Number: 1571-72-8

Molecular Formula: $C_7H_7NO_3$

Molecular Weight: 153.137

Accurate Mass: 153.042594

Percentage Composition: C 54.90%; H 4.61%; N 9.15%; O 31.34%

Physical Description: Yellow-amber prisms (H_2O)

Melting Point: Mp 201°. Mp 210°

pKa Value: pK_a 4.93

Aldrich: 28964-7

Fluka: 8110

>>Derivative: Hydrochloride

CAS Registry Number: 1571-65-9

Melting Point: Mp 275 dec.°

>>Derivative: Me ester

Synonym(s): Orthocaine. Orthoform New. Orthoderm

CAS Registry Number: 536-25-4

Molecular Formula: $C_8H_9NO_3$

Molecular Weight: 167.164

Accurate Mass: 167.058244

Percentage Composition: C 57.48%; H 5.43%; N 8.38%; O 28.71%

Use/Importance: Local anaesthetic (no longer in widespread use)

Physical Description: Light brown needles (C_6H_6 , AcOH, $CHCl_3$ or EtOH aq.)

Melting Point: Mp 142° (form 1). Mp 110-111° (90°) (form 2)

Calculated Log P Data: Log P 1.28 (calc)

Other Data: Dimorphic

>>Derivative: Et ester

Synonym(s): Anaesthaminol

CAS Registry Number: 13052-92-1

Molecular Formula: $C_9H_{11}NO_3$

Molecular Weight: 181.191

Accurate Mass: 181.073894

Percentage Composition: C 59.66%; H 6.12%; N 7.73%; O 26.49%

Use/Importance: Local anaesthetic

Physical Description: Dimorphic. Needles ($CHCl_3$ /petrol) or plates (EtOAc)

Melting Point: Mp 84°. Mp 112 resp.°

Calculated Log P Data: Log P 1.81 (calc)

>>Derivative: Amide

Molecular Formula: $C_7H_8N_2O_2$

Molecular Weight: 152.152

Accurate Mass: 152.058578

Percentage Composition: C 55.26%; H 5.30%; N 18.41%; O 21.03%

Physical Description: Tan solid

Melting Point: Mp 167-170°