



>>Entry Name: 5-Amino-2-hydroxybenzoic acid

Synonym(s): 5-Aminosalicylic acid. **Mesalazine**, BAN, INN. Mesalamine, USAN. Asacol. Asalit. Claversal. Fisalamine. Pentasa. Rowasa. Salofalk. 5-ASA. Many other names

CAS Registry Number: 89-57-6

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%

Use/Importance: Drug used for treatment of ulcerative colitis. Esters used as sunscreens. Antiinflammatory agent. Low acute oral toxicity

Physical Description: Needles ($NaHSO_3$ aq.)

Development Status: Launched 1984

Melting Point: Mp 283 dec.°

pKa Value: pK_{a1} 2.74; pK_{a2} 5.84

Calculated Log P Data: Log P 1.06 (calc)

Aldrich: A7980-9

Fluka: 9409

Sigma: A4283

>>Derivative: Me ester

CAS Registry Number: 42753-75-3

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%

Physical Description: Needles (C_6H_6)

Melting Point: Mp 96°

>>Derivative: Et ester

CAS Registry Number: 62773-65-3

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%

Physical Description: Needles (EtOH)

Melting Point: Mp 145°

>>Derivative: Amide

CAS Registry Number: 59393-77-0

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: Needles (NH_3 aq.)

Melting Point: Mp 194-197 dec.°

>>Derivative: Nitrile

Synonym(s): 2-Hydroxy-5-aminobenzonitrile. 4-Amino-2-cyanophenol

CAS Registry Number: 105430-53-3

Molecular Formula: $C_7H_6N_2O$

Molecular Weight: 134.137

Accurate Mass: 134.048013

Percentage Composition: C 62.68%; H 4.51%; N 20.88%; O 11.93%

Physical Description: Needles

Melting Point: Mp 160-162° (as hydrochloride)