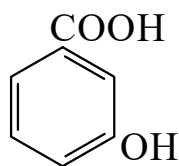




>>Entry Name: 3-Hydroxybenzoic acid, 9CI



CAS Registry Number: 99-06-9

Extra CAS Registry Numbers(s): 29656-58-4

Molecular Formula:  $C_7H_6O_3$

Molecular Weight: 138.123

Accurate Mass: 138.031695

Percentage Composition: C 60.87%; H 4.38%; O 34.75%

Biological Source: Isol. from plants, e.g. *Hydrangea macrophylla*, *Citrus paradisi*; present in fruits, prod. by *Penicillium griseofulvum*

Use/Importance: Monomer for polyesters

Physical Description: Needles ( $H_2O$ )

Melting Point: Mp 202°

Solubility: Sol.  $H_2O$ , hot EtOH

pKa Value:  $pK_a$  5.72 (25°, 50% EtOH aq.)  $pK_{a1}$  3.96;  $pK_{a2}$  9.61 (20°, 0.1M KCl)

Hazard & Toxicity: LD<sub>50</sub> (mus, orl) 2000 mg/kg. Exp. teratogenic effects (feto-embryotoxic)

Aldrich: H2000-8

Fluka: 54620

Sigma: H6761

>>Derivative: Me ester

CAS Registry Number: 19438-10-9

Molecular Formula:  $C_8H_8O_3$

Molecular Weight: 152.149

Accurate Mass: 152.047345

Percentage Composition: C 63.15%; H 5.30%; O 31.55%

Physical Description: Needles ( $C_6H_6$ /petrol)

Melting Point: Mp 71.5° (69°)

Boiling Point: Bp<sub>709</sub> 280-280.5°

Aldrich: 25279-4

Fluka: 54740

>>Derivative: Et ester

CAS Registry Number: 7781-98-8

Molecular Formula:  $C_9H_{10}O_3$

Molecular Weight: 166.176

Accurate Mass: 166.062995

Percentage Composition: C 65.05%; H 6.07%; O 28.88%

Physical Description: Plates ( $C_6H_6$ )

Melting Point: Mp 72-73°

Boiling Point: Bp 295°. Bp<sub>65</sub> 211°

pKa Value:  $pK_a$  9.1 (25°)

Aldrich: 25120-8

Fluka: 54650

>>Derivative: Isopropyl ester

CAS Registry Number: 53631-77-9

Molecular Formula:  $C_{10}H_{12}O_3$

Molecular Weight: 180.203

Accurate Mass: 180.078645

Percentage Composition: C 66.65%; H 6.71%; O 26.64%

Melting Point: Mp 59-60°

Boiling Point: Bp<sub>15</sub> 162-164°. Bp<sub>5</sub> 143-144°