



>>Entry Name: 4-Hydroxybenzaldehyde

ENTRY UNDER REVIEW

Synonym(s): *p*-Formylphenol



CAS Registry Number: 123-08-0

Related CAS Registry Numbers(s): 60221-52-5

Extra CAS Registry Numbers(s): 28777-87-9

Molecular Formula: C₇H₆O₂

Molecular Weight: 122.123

Accurate Mass: 122.03678

Percentage Composition: C 68.85%; H 4.95%; O 26.20%

Biological Source: Occurs naturally combined in many glycosides. Isol. free state from *Papaver somniferum*. Prod. by microorganisms. Present in sulfite liquor. Constit. of wing gland and abdominal hairpencils of the male African sugarcane borer *Eldana saccharina*

Use/Importance: Reagent for the colorimetric detn. of shikimic acid

Physical Description: Needles (H₂O)

Melting Point: Mp 115-116°

pK_a Value: pK_a 7.62 (25°, H₂O)

UV: [neutral] λ_{max} 221 (ε 12000); 284 (ε 14800); 291 () (MeOH) (Berdy) [neutral] λ_{max} 220 (ε 14800); 280 (ε 18700); 330 (ε 6600) (EtOH) (Berdy)

Aldrich: W50750-4

Fluka: 54590

Rare Chemicals Library: S10273-3

Sigma: H5630

>>Derivative: *O*-β-D-Glucopyranoside

Synonym(s): 4-Glucosyloxybenzaldehyde. **Hydrangea glucoside C**

CAS Registry Number: 26993-16-8

Molecular Formula: C₁₃H₁₆O₇

Molecular Weight: 284.265

Accurate Mass: 284.089605

Percentage Composition: C 54.93%; H 5.67%; O 39.40%

Biological Source: Constit. of *Hydrangea serrata*

Physical Description: Needles (EtOH)

Melting Point: Mp 168-170°

Optical Rotation: [α]_D¹⁶ -81.3 (c, 0.12 in MeOH)

>>Derivative: *O*-[4-Hydroxycinnamoyl-(→3 or 4)-β-D-glucopyranoside]

Synonym(s): **Nantenoside A**

CAS Registry Number: 54605-12-8

Molecular Formula: C₂₂H₂₂O₉

Molecular Weight: 430.41

Accurate Mass: 430.126385

Percentage Composition: C 61.39%; H 5.15%; O 33.46%

Biological Source: Constit. of the leaves of *Nandina domestica*

Physical Description: Yellow cryst. + 1H₂O

Melting Point: Mp 185-188°

>>Derivative: Oxime(*E*-)

Molecular Formula: C₇H₇NO₂

Molecular Weight: 137.138

Accurate Mass: 137.047679

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

Melting Point: Mp 115-116° (premelts from 106°)

Other Data: Readily forms a monohydrate. Synth. of anhyd. material requires careful drying