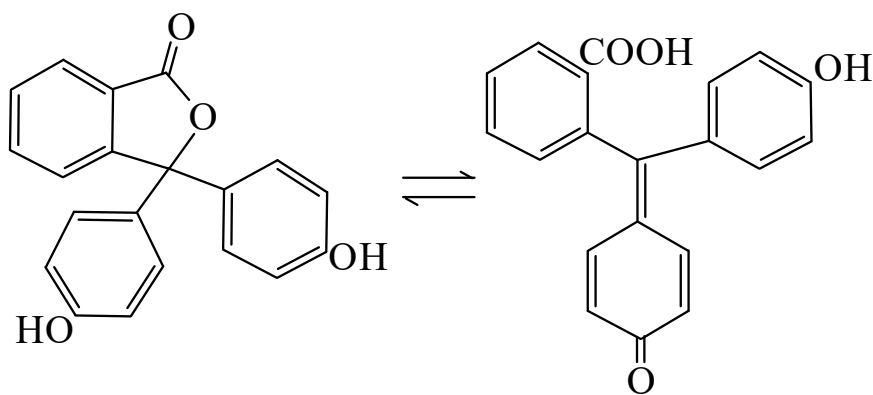




>>Entry Name: Phenolphthalein, BAN, INN

Synonym(s): 3,3-Bis(4-hydroxyphenyl)-1(3*H*)-isobenzofuranone, 9CI. 3,3-Bis(4-hydroxyphenyl)phthalide. α ,4,4'-Trihydroxytriphenylmethane-2-carboxylic acid lactone. Dihydroxyphthalophenone. Many other names



CAS Registry Number: 77-09-8

Related CAS Registry Numbers(s): 518-51-4 62625-16-5 84731-58-8

Molecular Formula: C₂₀H₁₄O₄

Molecular Weight: 318.328

Accurate Mass: 318.08921

Percentage Composition: C 75.46%; H 4.43%; O 20.10%

Use/Importance: Laxative. Used as EtOH soln. as an acid-base indicator (pH range 8.0-10) and in photometric detn. of CN⁽⁻⁾, Cl⁽⁻⁾, N₂H₄

Physical Description: Needles

Melting Point: Mp 258-262°

Solubility: Sol. EtOH, Et₂O; sl. sol. H₂O

Hazard & Toxicity: Hypersensitivity reactions and systemic effects reported when used therapeutically. Discolours urine or faeces pink or red

Aldrich: 31923-6

Fluka: 77622

Sigma: P9750

>>Derivative: Oxime

Molecular Formula: C₂₀H₁₅NO₄

Molecular Weight: 333.343

Accurate Mass: 333.100109

Percentage Composition: C 72.06%; H 4.54%; N 4.20%; O 19.20%

Melting Point: Mp 216°

>>Derivative: Me ester (open-chain form)

Molecular Formula: C₂₁H₁₆O₄

Molecular Weight: 332.355

Accurate Mass: 332.10486

Percentage Composition: C 75.89%; H 4.85%; O 19.26%

Physical Description: Orange-red needles

Melting Point: Mp 127-130°

>>Derivative: Et ester, Et ether (open-chain form)

Molecular Formula: C₂₄H₂₂O₄

Molecular Weight: 374.435

Accurate Mass: 374.15181

Percentage Composition: C 76.99%; H 5.92%; O 17.09%

Physical Description: Yellow cryst.

Melting Point: Mp 98-104°

>>Derivative: Di-Ac

CAS Registry Number: 5449-84-3

Molecular Formula: C₂₄H₁₈O₆

Molecular Weight: 402.403

Accurate Mass: 402.11034

Percentage Composition: C 71.64%; H 4.51%; O 23.86%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 146.5-147.3°