



>>Entry Name: Phenol

Synonym(s): Hydroxybenzene. Carbolic acid. Benzenol

CAS Registry Number: 108-95-2

Related CAS Registry Numbers(s): 100-67-4 2122-46-5 3229-70-7 5793-84-0 13127-88-3

PhOH

Molecular Formula: C₆H₆O

Molecular Weight: 94.113

Accurate Mass: 94.041865

Percentage Composition: C 76.57%; H 6.43%; O 17.00%

Biological Source: Minor constit. of plant oils in combined form. A major constit. of coal tar

Use/Importance: Used as 5% soln. in EtOH for photometric detn. of NO₃⁽⁻⁾; binding of Cl₂ and Br₂. Also used (with NaClO) for detn. of NH₃. Disinfectant. Used in manuf. of phenol-formaldehyde resins, bisphenol A, nylon intermediates and alkylphenols. Important industrial chemical, 33rd in order of volume for USA in 1994 (production 2.03 million tons/year)

Physical Description: Deliquescent needles with a characteristic odour

Melting Point: Mp 43°. Fp 41°

Boiling Point: Bp 181.8°. Bp₂₅ 90.2°

Solubility: Sol. H₂O, EtOH, Et₂O, Me₂CO, C₆H₆

Calculated Log P Data: Log P 1.47 (calc)

Other Data: Steam-volatile. Also used as sodium salt (Phenolate sodium, USAN)

Hazard & Toxicity: Fl. p. 75/79°, autoignition temp. 605/715°. OES: long-term 5 ppm; short-term 10 ppm (Sk). Violent reactions with a variety of substances. Vapour irritates respiratory system and eyes. Contact with solid or conc. solns. causes chemical burns of the skin and severe eye damage. Readily absorbed through skin and can cause headache, dizziness, respiratory distress, liver and kidney injury, and other effects. Fatalities recorded from skin absorption or ingestion

Aldrich: W32231-8

Fluka: 77613

Sigma: P4682

Supelco: R43-0650

>>Derivative: Na salt

Synonym(s): Phenolate sodium, USAN

Use/Importance: Disinfectant

Hazard & Toxicity: Corrosive and irritating to all tissues

>>Derivative: Picrate

Melting Point: Mp 83.1°

>>Derivative: Phenylurethane

Synonym(s): Hydroxyphenyl phenylcarbamate, 9CI

Molecular Formula: C₁₃H₁₁NO₂

Molecular Weight: 213.235

Accurate Mass: 213.078979

Percentage Composition: C 73.23%; H 5.20%; N 6.57%; O 15.01%

Physical Description: Needles (C₆H₆)

Melting Point: Mp 126°

>>Derivative: Hydrogen sulfate

Synonym(s): Sulfuric acid monophenyl ester, 9CI

CAS Registry Number: 937-34-8

Molecular Formula: C₆H₆O₄S

Molecular Weight: 174.177

Accurate Mass: 173.99868

Percentage Composition: C 41.38%; H 3.47%; O 36.74%; S 18.41%

Biological Source: Urinary metab. of phenol in man and animals

Other Data: Very unstable

>>Derivative: Formyl