4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of phenol is located in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of phenol is located in Table 4-2.
### Table 4-1. Chemical Identity of Phenol

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>Information</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemical name</td>
<td>Phenol</td>
<td>Lide 2005</td>
</tr>
<tr>
<td>Synonym(s)</td>
<td>Benzenol, hydroxybenzene, monophenol, oxybenzene, phenyl alcohol, phenyl hydrate, phenyl hydroxide, phenyllic acid, phenyllic alcohol</td>
<td>Lewis 2000</td>
</tr>
<tr>
<td>Registered trade name(s)</td>
<td>Carboxic acid, phenic acid, phenic alcohol</td>
<td>Gardner et al. 1978</td>
</tr>
<tr>
<td>Chemical formula</td>
<td>C₆H₅O</td>
<td>Lide 2005</td>
</tr>
<tr>
<td>Chemical structure</td>
<td><img src="" alt="Chemical structure" /></td>
<td>Budavari et al. 1989</td>
</tr>
</tbody>
</table>

Identification numbers:

- **CAS registry**: 108-95-2  
  HSDB 2008
- **NIOSH RTECS**: SJ3250000  
  RTECS 2006
- **EPA hazardous waste**: U188  
  EPA 1998; HSDB 2008
- **DOT/UN/NA/IMCO shipping**: UN 1671 (solid)  
  HSDB 2008
  UN 2312 (molten)  
  UN 2821 (solution)  
  IMO 6.1 (solid, molten, solution)
- **HSDB**: 113  
  HSDB 2008
- **NCI**: C50124  
  Lewis 2000

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; RTECS = Registry of Toxic Effects of Chemical Substances
### Table 4-2. Physical and Chemical Properties of Phenol

<table>
<thead>
<tr>
<th>Property</th>
<th>Information</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight</td>
<td>94.111</td>
<td>Lide 2005</td>
</tr>
<tr>
<td>Color</td>
<td>Colorless to light pink</td>
<td>HSDB 2008</td>
</tr>
<tr>
<td>Physical state</td>
<td>Crystalline solid liquid (w/ 8% H₂O)</td>
<td></td>
</tr>
<tr>
<td>Melting point</td>
<td>40.89 °C</td>
<td>Lide 2005</td>
</tr>
<tr>
<td>Boiling point</td>
<td>181.87 °C</td>
<td>Lide 2005</td>
</tr>
<tr>
<td>Density at 20 °C/4 °C</td>
<td>1.0545 at 45 °C/4 °C</td>
<td>Lide 2005</td>
</tr>
<tr>
<td>Vapor density</td>
<td>3.24</td>
<td>Lewis 2000</td>
</tr>
<tr>
<td>Odor</td>
<td>Distinct aromatic, somewhat sickening, sweet and acrid odor</td>
<td>HSDB 2008</td>
</tr>
<tr>
<td>Odor threshold:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water</td>
<td>7.9 ppm (w/v)</td>
<td>Amoore and Hautala 1983</td>
</tr>
<tr>
<td></td>
<td>1 ppm (w/v)</td>
<td>Baker et al. 1978</td>
</tr>
<tr>
<td>Air</td>
<td>0.040 ppm (v/v)</td>
<td>Amoore and Hautala 1983</td>
</tr>
<tr>
<td>Solubility:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water at 25 °C</td>
<td>8.28x10⁴ mg/L</td>
<td>Southworth and Keller 1986</td>
</tr>
<tr>
<td>Organic solvent(s)</td>
<td>Soluble in water and ethanol, very soluble in ether, miscible with acetone and benzene</td>
<td>Lide 2005</td>
</tr>
<tr>
<td>Partition coefficients:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Log K_{ow}</td>
<td>1.46</td>
<td>HSDB 2008</td>
</tr>
<tr>
<td>Log K_{oc}</td>
<td>1.21–1.96</td>
<td>Artiola-Fortuny and Fuller 1982; Boyd 1982; Briggs 1981; Sacan and Balcioglu 1996; Scott et al. 1983</td>
</tr>
<tr>
<td>Vapor pressure at 25 °C</td>
<td>0.35 mmHg</td>
<td>HSDB 2008</td>
</tr>
<tr>
<td>Henry's law constant</td>
<td>3.0x10⁻¹ atms m⁻³-mol</td>
<td>Gaffney et al. 1987</td>
</tr>
<tr>
<td>Autoignition temperature</td>
<td>715 °C</td>
<td>Lewis 2000</td>
</tr>
<tr>
<td>Flashpoint, open cup</td>
<td>85 °C</td>
<td>HSDB 2008</td>
</tr>
<tr>
<td>Flashpoint, closed cup</td>
<td>79 °C</td>
<td>HSDB 2008</td>
</tr>
<tr>
<td>Flammability limits (in air, by % v)</td>
<td>1.7–8.6%</td>
<td>HSDB 2008</td>
</tr>
<tr>
<td>Conversion factors:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ppm (v/v) to mg/m³ in air (25 °C)</td>
<td>ppm (v/v)x3.92=mg/m³</td>
<td></td>
</tr>
<tr>
<td>mg/m³ to ppm (v/v) in air (25 °C)</td>
<td>mg/m³x0.225=ppm (v/v)</td>
<td></td>
</tr>
</tbody>
</table>

atm = atmosphere; v = volume; w = weight