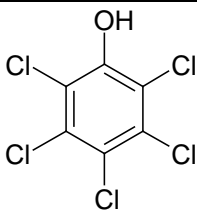
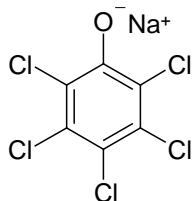


CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of pentachlorophenol is located in Table 4-1. A number of contaminants are found in commercial- and technical-grade pentachlorophenol formulations. Commonly found contaminants that were introduced during production include other chlorophenols, CDDs, CDFs, hexachlorobenzene, and chlorophenoxy compounds. Pure pentachlorophenol compounds are typically $\geq 98\%$ pure with very low levels of CDDs and CDFs. Commercial-grade pentachlorophenol is typically 90% pentachlorophenol, and technical-grade pentachlorophenol formulations typically contains 85–90% pentachlorophenol. A list of contaminants in technical-grade pentachlorophenol and two commercial-grade pentachlorophenol products (Dowicide EC-7 and DP-2) are presented in Table 2-1.

Table 4-1. Chemical Identity of Pentachlorophenol

Characteristic	Pentachlorophenol	Sodium pentachlorophenate
Synonym(s) and registered trade name(s)	PCP; penchlorol; penta; pentachlorophenate; 2,3,4,5,6-pentachlorophenol ^b	Pentachlorophenol sodium; pentachlorophenol sodium salt; pentachlorophenoxy sodium; pentaphenate
For 37% aqueous solution	Chlon; Dowicide 7; Dowicide EC-7; Dura Treet II; EP 30; Fungifen ^a	Dow Dormant Fungicide; Dowicide G; Dowicide
For polymeric form	Grundier Arbezol; Lauxtol; Liroprem; Penta Concentrate; Penta Ready; Penta WR; Permasan; Santophen 20; Woodtreat ^b	G-St; Mystox D; Napclor-G; Santobrite; Sapco25 Weedbeads
Chemical formula	C ₆ HCl ₅ O	C ₆ Cl ₅ ONa
Chemical structure		
CAS Registry Number	87-86-5	131-52-2

^aAll information obtained from HSDB 2001, except where noted.

CAS = Chemical Abstracts Service

4. CHEMICAL AND PHYSICAL INFORMATION

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of pentachlorophenol is located in Table 4-2.

Table 4-2. Physical and Chemical Properties of Pentachlorophenol

Property	Pentachlorophenol	Sodium pentachlorophenate
Molecular weight	266.34	288.34
Color	Colorless or white (pure); dark gray to brown (crude product)	White or tan
Physical state	Crystalline solid (pure); pellets or powder (crude product) ^b	Flakes or powder
Melting point	174°C	No data
Boiling point	309–310°C (decomposes)	No data
Density	1.978 g/mL at 22°C/4°C	2.0 mg/L at 22°C/4°C
Odor	Phenolic; very pungent (only when hot)	Phenolic odor
Odor threshold:		
Water	0.857 mg/L at 30°C; 12.0 mg/L at 60°C ^{b,c}	No data
Air	No data	No data
Solubility:		
Water	14 mg/L at 20°C	330,000 mg/L at 25°C
Organic solvents	Very soluble in alcohol and ether; soluble in benzene; slightly soluble in cold petroleum ether ^d	Soluble in acetone and ethanol
Partition coefficients:		
Log K _{ow}	5.01 ^b	No data
Log K _{oc}	4.5 ^e	No data
Vapor pressure at 20°C	0.00011 mmHg ^f	Not applicable
Dissociation constant (pKa)	4.70	Not applicable
Henry's law constant at 22°C	2.45x10 ⁻⁸ atm-m ³ /mol	Not applicable

^aAll information obtained from NLM (2021) unless otherwise noted.

^bVerschueren 1983.

^cHoak 1957.

^dBudavari et al. 1989.

^eSchellenberg et al. 1984.

^fEPA 1979.

^gLyman et al. 1982.