

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

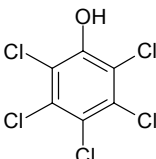
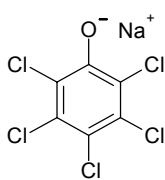
Information regarding the chemical identity of pentachlorophenol is located in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

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

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-1. Chemical Identity of Pentachlorophenol and Pentachlorophenate^a

Characteristic	Pentachlorophenol	Sodium pentachlorophenate
Synonym(s)	PCP; penchlorol; penta; pentachlorophenate; 2,3,4,5,6- pentachlorophenol ^b	Pentachlorophenol sodium; pentachlorophenol sodium salt; pentachlorophenoxy sodium; pentaphenate
Registered trade name(s) For 37% aqueous solution ^a	Chlon; Dovicide 7; Dovicide EC-7; Dura Treet II; EP 30;	Dow Dormant Fungicide; Dovicide G; Dovicide
For polymeric form ^b	Fungifen; 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		
Identification numbers:		
CAS Registry	87-86-5	131-52-2
NIOSH RTECS	SM6300000	SM6490000
EPA Hazardous Waste	U242; FO27	No data
OHM/TADS	7216842	No data
DOT/UN/NA/IMCO	NA 2020	UN 2567; IMO6.1
HSDB	894	761
NCI	C54933; C55378; C56655	No data

^aAll information obtained from HSDB 2001 except where noted.^bRTECS 1991

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 Substance Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-2. Physical and Chemical Properties of Pentachlorophenol and Sodium Pentachlorophenate^a

Property	Pentachlorophenol	Sodium pentachlorophenate
Molecular weight	266.35	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	190 EC	No data
Boiling point	309–310 EC (decomposes)	No data
Density	1.978 g/mL at 22 EC/4 EC	No data
Odor	Phenolic; very pungent (only when hot)	No data
Odor threshold: Water	0.857 mg/L at 30 EC; 12.0 mg/L at 60 EC ^{b,c}	No data
Solubility: Water	14 mg/L at 20 EC	330,000 mg/L at 25 EC
Organic solvent(s)	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 25 EC	0.00011 mmHg ^f	No data
Photolysis	t _{1/2} = 48 h ^g	t _{1/2} = 0.70 h ^h
Henry's law constant at 25 EC	3.4x10 ⁻⁶ atm-m ³ /mol ⁱ	No data
Autoignition temperature	No data	No data
Flashpoint	No data	No data
Flammability limits at 25 EC	No data	No data
Incompatibilities	No data	No data
Conversion factors (25 EC)	No data	No data
Explosive limits	No data	No data

^aAll information obtained from HSDB 2001 unless otherwise noted.

^bVerschueren 1983

^cHoak 1957

^dBudavari et al. 1989

^eSchellenberg et al. 1984

^fEPA 1979e

^gWong and Crosby 1981

^hPignatello et al. 1983

ⁱLyman et al. 1982