3. CHEMICAL AND PHYSICAL INFORMATION

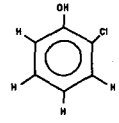
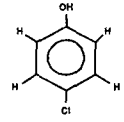
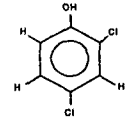
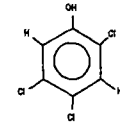
3.1 CHEMICAL IDENTITY

Information regarding the chemical identity of the chlorophenols is located in Table 3-l.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of the chlorophenols is located in Table 3-2. Except for 2-CP, which is a liquid at room temperature, all the chlorophenols discussed in this profile are solids at room temperature.

Table 3-1. Chemical Identity of Chlorophenol Compounds[a]

Characteristic	2-Chlorophenol	4-Chlorophenol	2,4-Dichlorophenol	2,4,5-Trichlorophenol
Synonym(s)	2-CP, 2 chloro-1-hydroxy-benzene, 2 hydroxy-chlorobenzene, *o*-chlorophenol, phenol	4-CP, 4-chloro-1-hydroxy-benzene, 4 hydroxy-chlorobenzene, *p*-chlorophenol, phenol	2,4-DCP, 2,4-dichlorohydroxybenzene	2,4,5-TCP
Registered trade name(s)	Sept-Kleen, Pine-O Disinfect	No data	No data	Preventol I, Collunosol
Chemical formula	C_6H_5ClO	C_6H_5ClO	$C_6H_4Cl_2O$	$C_6H_3Cl_3O$
Chemical structure				
Identification numbers:				
CAS registry	95-57-8	106-48-9	120-83-2	95-95-4
NIOSH RTECS	SK2625000	SK2800000	SR8575000	SN1400000
EPA hazardous waste	UO48	No data	UO51	DO41, FO27
OHM/TADS	8100049	81400051	7217235	8200170
DOT/UN/NA/IMCO shipping	UN 2020 liquid, IMO 6.1, UN 2021 solid	UN 2020 liquid, IMO 6.1, UN 2021 solid	UN 2020 solid, IMO 6.1	UN 2020, NA 2020, IMO 6.1
HSDB	1415	1414	1139	4067
NCI	No data	No data	C55346	C61187

[a]Data from HSDB 1994

CAS = Chemical Abstracts Service; 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; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

Table 3-1. Chemical Identity of Chlorophenol Compounds[a] (*continued*)

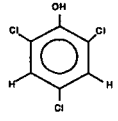
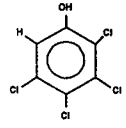
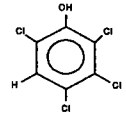
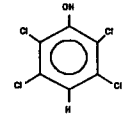
Characteristic	2,4,6-Trichlorophenol	2,3,4,5-Tetrachlorophenol	2,3,4,6-Tetrachlorophenol	2,3,5,6-Tetrachlorophenol
Synonyms	2,4,6-TCP	2,3,4,5-TeCP	2,3,4,6-TeCP	2,3,5,6-TeCP
Registered trade name(s)	Omal, Phenachlor	No data	No data	No data
Chemical formula	$C_6H_3Cl_3O$	$C_6H_2Cl_4O$	$C_6H_2Cl_4O$	$C_6H_2Cl_4O$
Chemical structure				
Identification numbers:				
CAS	88-06-2	4901-51-3	58-90-2	935-95-5
NIOSH RTECS	SN1575000	SM9200000	SM9275000	SM9450000
EPA hazardous waste	DO42, FO27	FO27	FO27	FO27
OHM/TADS	8200171	No data	8200152	No data
DOT/UN/NA/IMCO shipping	UN 2020, NA 2020 solid, IMO 6.1 solid	UN 2020, UN 2021, IMO 6.1	UN 2020 solid, UN 2021 liquid, IMO 6.1	UN 2020 solid, UN 2021 liquid, IMO 6.1
HSDB	4013	6765	1338	6766
NCI	C02904	No data	No data	No data

Table 3-2. Physical and Chemical Properties of Chlorophenol Compounds[a]

Property	2-Chlorophenol	4-Chlorophenol	2,4-Dichlorophenol	2,4,5-Trichlorophenol
Molecular weight	128.56	128.56	163.00	197.46
Color	Light amber	White to pink crystals	White	Gray
Physical state	Liquid	Solid	Solid	Solid
Melting point	9.3°C	43.2–43.7°C	45°C	67°C
Boiling point	174.9°C at 760 mmHg	220°C	210°C	235°C
Density	1.2634	1.2238 at 78°C/4°C	1.383 at 60°C/25°C	1.678 at 25°C/4°C
Odor	Unpleasant, medicinal odor	Medicinal odor	Strong medicinal odor	Strong phenolic odor
Odor threshold:				
Water at 30°C[b]	0.33 µg/L	0.33 µg/L	0.35 µg/L	11 µg/L
Air[c]	0.0189 mg/m^3	0.0189 mg/m^3	1.40 mg/m^3	No data
Solubility:				
Water at 25°C[d]	20,000 ppm	27,000 ppm	4,500 ppm	948 ppm
Organic solvent(s)	Acetone, alcohol, benzene	Alcohol, glycerol, ether, chloroform, fixed and volatile oils, benzene	Ethyl alcohol, carbon tetrachloride, ethyl ether, benzene, chloroform	Acetone, benzene, carbon tetrachloride, ether, denatured alcohol, methanol, liquid petrolatum, toluene
Other solvent(s)	Sodium hydroxide			
pK_a[d]	8.49	8.85	7.68	7.43
Partition coefficients:				
Log K_{ow}[d]	2.17	2.4	3.2	3.72
Log K_{oc}[d]	1.25–3.7	1.2–2.7	2.42–3.98	2.55–3.98
Vapor pressure at 25°C (liquid)[d]	0.99 mmHg	0.23 mmHg	0.14 mmHg	0.05 mmHg
(solid)[d]	0.99 mmHg	0.15 mmHg	0.09 mmHg	0.02 mmHg
Henry's law constant at 25°C[d]	6.8×10^{-6} atm-m^3/mol	9.2×10^{-7} atm-m^3/mol	4.3×10^{-6} atm-m^3/mol	5.1×10^{-6} atm-m^3/mol
Autoignition temperature	No data	No data	No data	No data
Flashpoint	64°C	121°C	114°C	No data
Flammability limits	No data	No data	No data	No data
Conversion factors (ppm to mg/m^3)	2.2	1.1	1.1	No data
Explosive limits	No data	No data	No data	No data

[a]Data from HSDB 1994 except where indicated
[b]From Hoak 1957
[c]From Ruth 1986
[d]From Shiu et al. 1994

Table 3-2. Physical and Chemical Properties of Chlorophenol Compounds[a] (*continued*)

Property	2,4,6-Trichlorophenol	2,3,4,5-Tetrachlorophenol	2,3,4,6-Tetrachlorophenol	2,3,5,6-Tetrachlorophenol
Molecular weight	197.45	231.89	231.89	231.89
Color	Yellow	No data	Light brown	No data
Physical state	Solid	Solid	Solid	Solid
Melting point	69°C	116–117°C	70°C	115°C
Boiling point	246°C	Sublimes	64°C	No data
Density	1.4901	No data	1.83 at 25°C/4°C	No data
Odor	Strong phenolic odor	No data	Strong odor	No data
Odor threshold:				
Water at 30°C[b]	100 µg/L	No data	915 µg/L	No data
Air[c]	No data	No data	No data	No data
Solubility:				
Water at 25°C[d]	434 ppm	166 ppm	183 ppm	100 ppm
Organic Solvent(s)	Acetone, benzene, carbon tetrachloride, diacetone alcohol, methanol, stoddard solvent, touene, turpentine, ether	Alcohol	Acetone, alcohol, benzene, chloroform, ligroin	Benzene
Other Solvent(s)	Hot acetic acid		Hot acetic acid, sodium hydroxide	
pK_a[d]	7.42	6.96	5.38	5.48
Partition coefficients:				
Log K_{ow}[d]	3.69	4.8	4.45	4.9
Log K_{oc}[d]	1.94–3.34	2.9–4.14	3.2–4.21	No data
Vapor pressure at 25°C (liquid)[d]	0.03 mmHg	0.0059 mmHg	0.0059 mmHg	0.0059 mmHg
(solid)[d]	0.0094 mmHg	0.0008 mmHg	0.0021 mmHg	0.0008 mmHg
Henry's law constant at 25°C[d]	5.7×10^{-6} atm-m^3/mol	1.3×10^{-6} atm-m^3/mol	3.6×10^{-6} atm-m^3/mol	2.2×10^{-6} atm-m^3/mol
Autoignition temperature	No data	No data	No data	No data
Flashpoint	No data	No data	No data	No data
Flammability limits	No data	No data	No data	No data
Conversion factors (ppm to mg/m^3)	No data	No data	No data	No data
Explosive limits	No data	No data	No data	No data