

CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

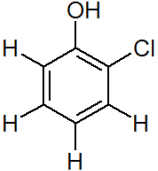
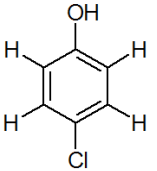
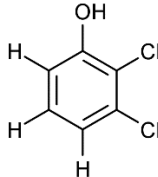
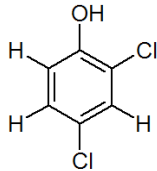
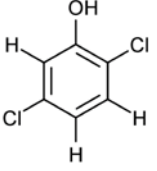
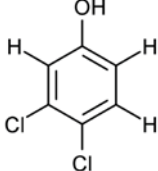
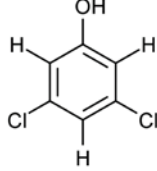
Information regarding the chemical identity of the chlorophenols is located in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of the chlorophenols is located in Table 4-2. Except for 2-CP, which is a liquid at room temperature, all of the chlorophenols discussed in this profile are solids at room temperature.

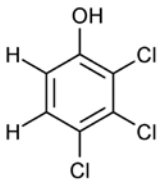
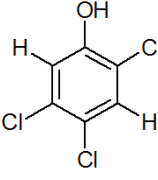
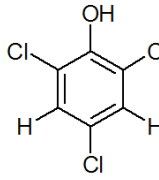
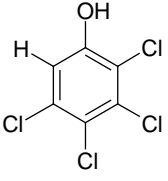
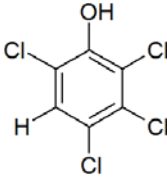
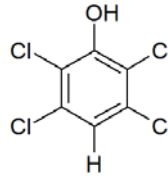
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Table 4-1. Chemical Identity of Chlorophenol Compounds

Characteristic		Information		
Chemical name	2-Chlorophenol	4-Chlorophenol	2,3-Dichlorophenol	2,4-Dichlorophenol
Synonym(s) and registered trade name(s)	2-CP, 2-chloro-1-hydroxybenzene, 2-hydroxychlorobenzene, <i>o</i> -chlorophenol	4-CP, 4-chloro-1-hydroxybenzene, 4-hydroxychlorobenzene, <i>p</i> -chlorophenol	2,3-DCP	2,4-DCP, 2,4-dichlorohydroxybenzene
Chemical formula	C ₆ H ₅ ClO	C ₆ H ₅ ClO	C ₆ H ₄ Cl ₂ O	C ₆ H ₄ Cl ₂ O
Chemical structure				
CAS Registry Number	95-57-8	106-48-9	576-24-9	120-83-2
Characteristic		Information		
Chemical name	2,5-Dichlorophenol	3,4-Dichlorophenol	3,5-Dichlorophenol	
Synonym(s) and registered trade name(s)	2,5-DCP, 2,5-dichloro-1-hydroxybenzene, 1-Hydroxy-2,5-dichlorobenzene	3,4-DCP, 4,5-dichlorophenol	3,5-DCP, 1-Hydroxy-3,5-dichlorobenzene	
Chemical formula	C ₆ H ₄ Cl ₂ O	C ₆ H ₄ Cl ₂ O	C ₆ H ₄ Cl ₂ O	
Chemical structure				
CAS Registry Number	583-78-8	95-77-2	591-35-5	

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Table 4-1. Chemical Identity of Chlorophenol Compounds

Characteristic		Information		
Chemical name	2,3,4-Trichlorophenol	2,4,5-Trichlorophenol	2,4,6-Trichlorophenol	
Synonym(s) and registered trade name(s)	2,3,4-TCP	2,4,5-TCP	2,4,6-TCP, Omal, Phenachlor	
Chemical formula	C ₆ H ₃ Cl ₃ O	C ₆ H ₃ Cl ₃ O	C ₆ H ₃ Cl ₃ O	
Chemical structure				
CAS Registry Number	15950-66-0	95-95-4	88-06-2	
Characteristic		Information		
Chemical name	2,3,4,5-Tetrachlorophenol	2,3,4,6-Tetrachlorophenol	2,3,5,6-Tetrachlorophenol	
Synonym(s) and registered trade name(s)	2,3,4,5-TeCP	2,3,4,6-TeCP	2,3,5,6-TeCP	
Chemical formula	C ₆ H ₂ Cl ₄ O	C ₆ H ₂ Cl ₄ O	C ₆ H ₂ Cl ₄ O	
Chemical structure				
CAS Registry Number	4901-51-3	58-90-2	935-95-5	

CAS = Chemical Abstracts Service

Sources: NLM (2003a, 2003b, 2003c, 2009a, 2009b, 2009c, 2015, 2019, 2020a, 2020b, 2020c, 2020d, 2020e)

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Table 4-2. Physical and Chemical Properties of Chlorophenol Compounds^a

Characteristic	2-Chlorophenol	4-Chlorophenol	2,3-Dichlorophenol	2,4-Dichlorophenol
Molecular weight	128.56	128.56	163.00	163.00
Color	Light amber	White to pink crystals	Brown	White
Physical state	Liquid	Solid	Solid	Solid
Melting point	9.3°C	43.2–43.7°C	58°C	45°C
Boiling point	174.9°C	220°C	206°C	210°C
Density at 20°C	1.2634	1.2238 at 78°C/4°C	No data	1.383 at 60°C/25°C
Odor	Unpleasant, medicinal odor	Medicinal odor	No data	Strong medicinal odor
Odor threshold:				
Water at 30°C ^b	0.33 µg/L	33 µg/L	No data	0.65 µg/L
Air ^c	0.0189 mg/m ³	0.0189 mg/m ³	No data	1.40 mg/m ³
Solubility:				
Water at 25°C ^d	20,000 ppm	27,000 ppm at pH 5.1	8,215 ppm at pH 4.9	4,500 ppm
Organic solvents	Acetone, alcohol, benzene	Alcohol, glycerol, ether, chloroform, fixed and volatile oils, benzene	Alcohol, ethyl ether, benzene, ligroin	Alcohol, carbon tetrachloride, ethyl ether, benzene, chloroform
Partition coefficients:				
Log K _{ow}	2.17 ^d	2.4 ^d	2.84	3.06
Log K _{oc} ^d	1.25–3.7	1.2–2.7	2.63	2.42–3.98
Vapor pressure at 25°C ^d	0.99 mmHg at 25°C	0.23 mmHg at 25°C	0.058 mmHg at 25°C ^a	0.14 mmHg at 25°C
Henry's law constant at 25°C ^d	6.8x10 ⁻⁶ atm-m ³ /mol	9.2x10 ⁻⁷ atm-m ³ /mol	1.6x10 ⁻⁶ atm-m ³ /mol (calculated)	4.3x10 ⁻⁶ atm-m ³ /mol
pK _a ^f	8.52	9.37	7.71	7.90
Autoignition temperature	No data	No data	No data	No data
Flashpoint	64°C	121°C	No data	114°C
Flammability limits	No data	No data	No data	No data
Conversion factors	1 ppm=5.3 mg/m ³ at 25°C, 1 atm	1 ppm=5.3 mg/m ³ at 25°C, 1 atm	1 ppm=6.7 mg/m ³ at 25°C, 1 atm	1 ppm=6.7 mg/m ³ at 25°C, 1 atm
Explosive limits	No data	No data	No data	No data

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Table 4-2. Physical and Chemical Properties of Chlorophenol Compounds^a

Characteristic	2,5-Dichlorophenol	3,4-Dichlorophenol	3,5-Dichlorophenol
Molecular weight	163.00	163.00	163.00
Color	White	Brown or yellow	Pink
Physical state	Solid	Solid	Solid
Melting point	59°C	68°C	68°C
Boiling point	211°C	253°C	233°C
Density at 20°C	No data	No data	No data
Odor	No data	No data	No data
Odor threshold:			
Water at 30°C ^b	3.3 µg/L	No data	No data
Air ^c	No data	No data	No data
Solubility:			
Water at 25°C ^d	2,000 ppm at unknown pH ^a	9,256 ppm at pH 5.1	7,394 ppm at pH 4.7
Organic solvents	Alcohol, ethyl ether, benzene, petroleum ether	Alcohol, ethyl ether, benzene, petroleum ether	Alcohol, ethyl ether, petroleum ether
Partition coefficients:			
Log K _{ow}	3.06	3.33	3.62
Log K _{oc}	2.78 (estimated) ^e	2.93 (estimated) ^e	3.1 (estimated) ^e
Vapor pressure at 25°C	0.0562 mmHg at 25°C	0.00173 mmHg at 25°C (estimated) ^e	0.00842 mmHg at 25°C ^d
Henry's law constant at 25°C	6.0x10 ⁻⁶ atm-m ³ /mol (calculated) ^d	3.1x10 ⁻⁷ atm-m ³ /mol (estimated) ^e	2.4x10 ⁻⁷ atm-m ³ /mol (calculated) ^d
pK _a ^f	7.51	8.62	8.25
Autoignition temperature	No data	No data	No data
Flashpoint	No data	No data	No data
Flammability limits	No data	No data	No data
Conversion factors	1 ppm=6.7 mg/m ³ at 25°C, 1 atm	1 ppm=6.7 mg/m ³ at 25°C, 1 atm	1 ppm=6.7 mg/m ³ at 25°C, 1 atm
Explosive limits	No data	No data	No data

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Table 4-2. Physical and Chemical Properties of Chlorophenol Compounds^a

Characteristic	2,3,4-Trichlorophenol	2,4,5-Trichlorophenol	2,4,6-Trichlorophenol
Molecular weight	197.45	197.46	197.45
Color	Peach	Gray	Yellow
Physical state	Solid	Solid	Solid
Melting point	83.5°C	67°C	69°C
Boiling point	252°C	235°C	246°C
Density at 20°C	No data	1.678 at 25°C/4°C	1.4901
Odor	Strong disinfectant odor	Strong phenolic odor	Strong phenolic odor
Odor threshold:			
Water at 30°C ^b	No data	11 µg/L	100 µg/L
Air ^c	No data	No data	No data
Solubility:			
Water at 25°C ^d	915 ppm at pH 5.1	948 ppm at pH 5.1	434 ppm at pH 5.1
Organic solvents	No data	Acetone, benzene, carbon tetrachloride, ether, denatured alcohol, methanol, liquid petroleum, toluene	Acetone, benzene, carbon tetrachloride, diacetone alcohol, methanol, Stoddard solvent, toluene, turpentine, ether
Partition coefficients:			
Log K _{ow} ^d	3.80	3.72	3.69
Log K _{oc} ^d	No data	2.55–3.98	1.94–3.34
Vapor pressure at 25°C ^d	0.0027 mmHg at 25°C (estimated)	0.05 mmHg at 25°C	0.03 mmHg at 25°C
Henry's law constant at 25°C	3.9x10 ⁻⁶ atm-m ³ /mol ^d	2.21x10 ⁻⁶ atm-m ³ /mol (estimated) ^e	6.8x10 ⁻⁶ atm-m ³ /mol ^d
pK _a ^f	6.97	6.72	5.99
Autoignition temperature	No data	No data	No data
Flashpoint	62°C	No data	64°C
Flammability limits	No data	No data	No data
Conversion factors	1 ppm=8.1 mg/m ³ at 25°C, 1 atm	1 ppm=8.1 mg/m ³ at 25°C, 1 atm	1 ppm=8.1 mg/m ³ at 25°C, 1 atm
Explosive limits	No data	No data	No data

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Table 4-2. Physical and Chemical Properties of Chlorophenol Compounds^a

Characteristic	2,3,4,5-Tetrachlorophenol	2,3,4,6-Tetrachlorophenol	2,3,5,6-Tetrachlorophenol
Molecular weight	231.89	231.89	231.89
Color	No data	Light brown	No data
Physical state	Solid	Solid	Solid
Melting point	116–117°C	70°C	115°C
Boiling point	Sublimes	64°C	No data
Density at 20°C	No data	1.83 at 25°C/4°C	No data
Odor	No data	Strong odor	No data
Odor threshold:			
Water at 30°C ^b	No data	915 µg/L	No data
Air ^c	No data	No data	No data
Solubility:			
Water at 25°C ^d	166 ppm at pH 4.9	183 ppm at pH 5.3	100 ppm at pH 5.0
Organic solvents	Alcohol	Acetone, alcohol, benzene, chloroform, ligroin	Benzene
Partition coefficients:			
Log K _{ow} ^d	4.8	4.45	4.9
Log K _{oc} ^d	2.9–4.14	3.2–4.21	No data
Vapor pressure at 25°C ^d	0.0059 mmHg at 25°C	0.0059 mmHg at 25°C	0.0059 mmHg at 25°C
Henry's law constant at 25°C	3.5x10 ⁻⁷ atm-m ³ /mol (estimated) ^e	4.3x10 ⁻⁶ atm-m ³ /mol ^d	5.1x10 ⁻⁶ atm-m ³ /mol ^d
pK _a ^f	5.64	5.22	5.03
Autoignition temperature	No data	No data	No data
Flashpoint	121°C	114°C	No data
Flammability limits	No data	No data	No data
Conversion factors	1 ppm=9.5 mg/m ³ at 25°C, 1 atm	1 ppm=9.5 mg/m ³ at 25°C, 1 atm	1 ppm=9.5 mg/m ³ at 25°C, 1 atm

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Table 4-2. Physical and Chemical Properties of Chlorophenol Compounds^a

Characteristic	2,3,4,5-Tetrachlorophenol	2,3,4,6-Tetrachlorophenol	2,3,5,6-Tetrachlorophenol
Explosive limits	No data	No data	No data

^aData from NLM (2003a, 2003b, 2003c, 2009a, 2009b, 2009c, 2015, 2019, 2020a, 2020b, 2020c, 2020d, 2020e) except where noted.

^bHoak 1957.

^cRuth 1986.

^dShiu et al. 1994.

^eEPA 2012.

^fMuller and Caillard 2011.