

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

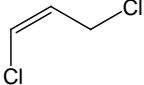
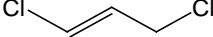
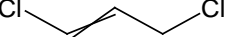
Data pertaining to the chemical identity of 1,1-, 1,2-, cis-1,3-, trans-1,3-, 2,3-, and 3,3-dichloropropene are listed in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

The physical and chemical properties of 1,1-, 1,2-, cis-1,3-, trans-1,3-, 2,3-, and 3,3-dichloropropene are presented in Table 4-2.

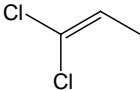
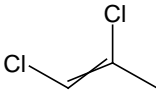
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Table 4-1. Chemical Identity of the Isomers of Dichloropropene

Characteristics	cis-1,3-Dichloropropene	trans-1,3-Dichloropropene	cis- and trans-1,3-Dichloropropene	References
Chemical name	cis-1,3-Dichloropropene	trans-1,3-Dichloropropene	1,3-Dichloropropene	Lide 2005; NIOSH 2005
Synonyms	(Z)-1,3-Dichloropropene; cis-1,3-dichloro-1-propene; cis-1,3-dichloro-propylene; cis-DCP	(E)-1,3-Dichloropropene; trans-1,3-dichloro-1-propene; trans-1,3-dichloro-propylene; trans-DCP	1,3-Dichloropropene; 1,3-dichloro-1-propene; 1,3-dichloro-propylene; 1,3-D	ChemID 2006a, 2006b
Trade names	Not applicable	Not applicable	PIC CLOR; TRICAL; TRI-CAL TRILONE II; TRI-FORM; TELONE; INLINE	EPA 2006i
Chemical formula	C ₃ H ₄ Cl ₂	C ₃ H ₄ Cl ₂	C ₃ H ₄ Cl ₂	RTECS 2006
Chemical structure				ChemID 2006a, 2006b; Lemen 2001; Lide 2005;
Identification numbers:				
CAS registry	10061-01-5	10061-02-6	542-75-6	RTECS 2006
NIOSH RTECS	UC8325000	UC8320000	UC8310000	RTECS 2006
EPA hazardous waste	Not available	Not available	U084	RTECS 2006
DOT/UN/NA/IMCO shipping	UN/DOT 2047; IMO 3.2	UN/DOT 2047; IMO 3.2	UN/DOT 2047; IMO 3.3	DOT 2000; HSDB 2006
HSDB	1503	1504	1109	HSDB 2006
NCI	Not available	Not available	NCI-C03985	HSDB 2006

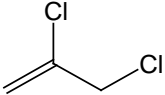
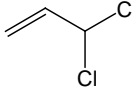
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Table 4-1. Chemical Identity of the Isomers of Dichloropropene

Characteristics	1,1-Dichloropropene	1,2-Dichloropropene	References
Chemical name	1,1-Dichloropropene	1,2-Dichloropropene	ChemID 2006c, 2006d; Lide 2005; RTECS 2006
Synonyms	1,1-Dichloro-1-propene; propene, 1,1-dichloro-; 1,1-dichloropropylene	Propene, 1,2-dichloro-; 1,2-dichloropropylene; propylene dichloride	ChemID 2006c, 2006d; RTECS 2006
Trade names	Not applicable	Not applicable	
Chemical formula	C ₃ H ₄ Cl ₂	C ₃ H ₄ Cl ₂	RTECS 2006
Chemical structure			ChemID 2006c, 2006d; Lide 2005
Identification numbers:			
CAS registry	563-58-6	563-54-2	RTECS 2006
NIOSH RTECS	UC8290000	UC8300000	RTECS 2006
EPA hazardous waste	Not available	Not available	RTECS 2006
DOT/UN/NA/IMCO shipping	UN/DOT 2047; IMO not available	UN/DOT 2047; IMO 3.3	DOT 2000; HSDB 2006
HSDB	Not applicable	6175	HSDB 2006
NCI	Not available	Not available	HSDB 2006

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Table 4-1. Chemical Identity of the Isomers of Dichloropropene

Characteristics	2,3-Dichloropropene	3,3-Dichloropropene	References
Chemical name	2,3-Dichloropropene	3,3-Dichloropropene	ChemID 2006e, 2006f; Lide 2005;
Synonyms	2,3-Dichloro-1-propene; 1,2-dichloro-2-propene; propene, 2,3-dichloro-; 2,3-dichloropropylene	1-Propene, 3,3-dichloro	ChemID 2006e, 2006f
Trade names	Not applicable	Not applicable	
Chemical formula	C ₃ H ₄ Cl ₂	C ₃ H ₄ Cl ₂	ChemID 2006e, 2006f
Chemical structure			ChemID 2006e, 2006f
Identification numbers:			
CAS registry	78-88-6	563-57-5	ChemID 2006e, 2006f
NIOSH RTECS	UC8400000	Not applicable	HSDB 2006
EPA hazardous waste	Not available	Not available	
DOT/UN/NA/IMCO shipping	UN/DOT 2047; IMO 3.3	UN/DOT 2047; IMO not available	DOT 2000
HSDB	5222	Not applicable	HSDB 2006
NCI	Not available	Not available	

CAS = Chemical Abstracts Service; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/Intergovernmental Maritime Consultative Organization; EPA = Environmental Protection Agency; HSDB = Hazardous Substance Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; RTECS = Registry of Toxic Effects of Chemical Substances

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Table 4-2. Physical and Chemical Properties of the Isomers of Dichloropropene

Property	cis-1,3-Dichloropropene	trans-1,3-Dichloropropene	cis- and trans-1,3-Dichloropropene	References
Molecular weight	110.97	110.97	110.97	RTECS 2006
Color	Colorless	Colorless	Colorless to amber	Lewis 2001; Tomlin 2003
Physical state	Liquid	Liquid	Liquid	Lewis 2001; Tomlin 2003
Melting point	Not available	Not available	-84 °C	Verschueren 2001
Boiling point	104.3 °C	112.0 °C	108 °C	O'Neil et al. 2001
Density	1.224 g/cm ³ at 20 °C	1.217 g/cm ³ at 20 °C	1.211 g/cm ³ at 25 °C	Meister et al. 2006; O'Neil et al. 2001
Odor	Not available	Not available	Sweet, penetrating	Tomlin 2003
Odor threshold				
Water	Not available	Not available	Not available	
Air	Not available	Not available	1 ppm	Verschueren 2001
Solubility				
Water at 20 °C	2.7x10 ³ mg/L	2.8x10 ³ mg/L	2.0x10 ³ mg/L	Dilling 1977; Tomlin 2003
Organic solvents	Soluble in ether, benzene, and chloroform	Soluble in ether, benzene, and chloroform	Miscible with hydrocarbons, halogenated solvents, esters, and ketones	Lide 2005; Tomlin 2003
Partition coefficients				
Log octanol/water	2.06	2.03	1.82	Tomlin 2003
K _{oc}	23, 25.7, 26.3, 27.6	26, 27.8, 27.2, 27.5	18–60	Hamaker and Thompson 1972; Kenaga 1980; Kim et al. 2003b
Vapor pressure	30 mm Hg at 20 °C	22 mm Hg at 20 °C	27.8 mm Hg at 20 °C	Dilling 1977; EPA 1981c
Vapor density (air = 1)	Not available	Not available	3.83	Lemen 2001
Henry's law constant (atm/m ³ -molecule at 20 °C)	2.71x10 ⁻³	8.71x10 ⁻⁴	3.55x10 ⁻³	EPA 1987b; Leistra 1970
Flashpoint (open cup)	21 °C (69.8 °F)	21 °C (69.8 °F)	35 °C (95 °F)	Lewis 2000, 2001
Conversion factors				
ppm (v/v) to mg/m ³ in air (20 °C)	4.61	4.61	4.61	Verschueren 2001
mg/m ³ to ppm (v/v) in air (20 °C)	0.22	0.22	0.22	Verschueren 2001
Bioconcentration factor (log BCF)	Not available	Not available	Not available	
Explosive limits	Not available	Not available	5.3–14.5%	NIOSH 2005

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Table 4-2. Physical and Chemical Properties of the Isomers of Dichloropropene

Property	1,1-Dichloropropene	1,2-Dichloropropene	References
Molecular weight	110.97	110.97	RTECS 2006
Color	Not available	Not available	
Physical state	Liquid	Liquid	EPA 1981c
Melting point	Not available	Not available	
Boiling point	76.5 °C	75 °C	Lide 2005; Verschueren 2001
Density	1.186 g/cm ³ at 25 °C	Not available	Lide 2005
Odor	Not available	Not available	
Odor threshold			
Water	Not available	Not available	
Air	Not available	Not available	
Solubility			
Water at	Not available	2.7x10 ³ mg/L at 25 °C	Gunther et al. 1968
Organic solvents	Soluble in ether, acetone, and chloroform	Soluble in ether, benzene, and chloroform	Lide 2005
Partition coefficients			
Log octanol/water	Not available	Not available	
K _{oc}	Not available	Not available	
Vapor pressure	91 mm Hg at 20 °C	91 mm Hg at 20 °C	EPA 1981c
Vapor density (air=1)	Not available	3.83	Lewis 2000; Verschueren 2001
Henry's law constant (atm/m ³ -molecule at 20 °C)	Not available	Not available	
Flashpoint	Not available	Not available	
Conversion factors			
ppm (v/v) to mg/m ³ in air (20 °C)	4.61	4.61	Verschueren 2001
mg/m ³ to ppm (v/v) in air (20 °C)	0.22	0.22	Verschueren 2001
Bioconcentration factor (log BCF)	Not available	Not available	
Explosive limits	Not available	Not available	

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Table 4-2. Physical and Chemical Properties of the Isomers of Dichloropropene

Property	2,3-Dichloropropene	3,3-Dichloropropene	References
Molecular weight	110.97	110.97	ChemID 2006e, 2006f; RTECS 2006
Color	Straw-colored	Not available	Verschueren 2001
Physical state	Liquid	Liquid	EPA 1981c; Lide 2005
Melting point	10 °C	Not available	Lide 2005; Verschueren 2001
Boiling point	94 °C	84.4 °C	EPA 1981c; Lide 2005
Density (20 °C)	1.211 g/cm ³ at 20 °C	1.224 g/cm ³ at 20 °C	Lide 2005; Meister et al. 2006; O'Neil et al. 2001
Odor	Pungent	Not available	Verschueren 2001
Odor threshold			
Water	Not available	Not available	
Air	Not available	Not available	
Solubility			
Water	2.15x10 ³ mg/L at 25 °C	Not available	Mackay and Shiu 1981
Organic solvents	Miscible in ethanol, soluble in ether, benzene, and chloroform	Soluble in ether, benzene, and chloroform	Lide 2005; Tomlin 2003
Partition coefficients			
Log octanol/water	Not available	Not available	
K _{oc}	Not available	Not available	
Vapor pressure	45 mm Hg at 20 °C	71 mm Hg at 20 °C	EPA 1981c
Vapor density (air=1)	3.8	Not available	Lewis 2000; Verschueren 2001
Henry's law constant (atm/m ³ -molecule at 20 °C)	Not available	Not available	
Flashpoint	10 °C (50 °F)	Not available	Lewis 2000
Conversion factors			
ppm (v/v) to mg/m ³ in air (20 °C)	4.61	4.61	Verschueren 2001
mg/m ³ to ppm (v/v) in air (20 °C)	0.22	0.22	Verschueren 2001
Bioconcentration factor (log BCF)	Not available	Not available	
Explosive limits	Not available	Not available	