CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

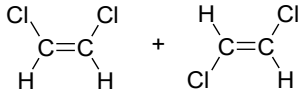
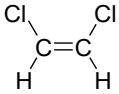
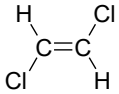
4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of 1,2-dichloroethene is in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of 1,2-dichloroethene is in Table 4-2. There are two geometric isomers of 1,2-dichloroethene: the cis- form and the trans- form. The two are often used as a mixture, which typically contains more trans-1,2-dichloroethene. Both cis- and trans-1,2-dichloroethene are low molecular weight organochlorides with high vapor pressures and vapor densities heavier than air (NLM 2022a, 2022b).

Table 4-1. Chemical Identity of Isomers of 1,2-Dichloroethene

Characteristic	Information[a]		
Chemical name	1,2-Dichloroethene	cis-1,2-Dichloroethene	trans-1,2-Dichloroethene
Synonym(s) and registered trade name(s)	Acetylene dichloride; 1,2-Dichloroethylene; sym-1,2-Dichloroethylene; 1,2-DCE; Dioform[b]	(Z)-1,2-Dichloroethene; (Z)-1,2-Dichloroethylene; cis-Acetylene dichloride; cis-1,2-Dichloroethylene; cis-Dichloroethylene	(E)-1,2-Dichloroethene; (E)-1,2-Dichloroethylene; trans-Acetylene dichloride; trans-1,2-Dichloroethylene; trans-Dichloroethylene
Chemical formula	$C_2H_2Cl_2$	$C_2H_2Cl_2$	$C_2H_2Cl_2$
Chemical structure			
CAS Registry Number	540-59-0	156-59-2	156-60-5

[a]All information from NLM (2022a; cis-1,2-dichloroethene) and NLM (2022b; trans-1,2-dichloroethene), except where noted.
[b]Bennett 1981.

CAS = Chemical Abstracts Services

Table 4-2. Physical and Chemical Properties of cis- and trans-1,2-Dichloroethene

Property	cis-1,2-Dichloroethene	trans-1,2-Dichloroethene	Reference
Molecular weight	96.95	96.95	NLM 2022a, 2022b
Color	Colorless	Colorless	NLM 2022a, 2022b
Physical state	Liquid	Liquid	Hawley 1981; NLM 2022a, 2022b
Melting point	-80.0°C	-49.8°C	NLM 2022a, 2022b
Boiling point	58–60°C at 760 mmHg	47–49°C at 760 mmHg	NLM 2022a, 2022b
Density (g/cm^3)	1.2837	1.2565	NLM 2022a, 2022b
Odor	Sweetish	Sweetish	NLM 2022a, 2022b
Odor threshold:			
Water	No data	No data	
Air	No data	Odor low: 0.3357 mg/m^3; odor high 1,975.00 ppm	NLM 2022b
Solubility:			
Water (at 25°C)	1–5 mg/mL; 6,410 mg/L at 25°C	4,520 mg/L at 25°C	NLM 2022a, 2022b
Organic solvents	Soluble in ether, alcohol, benzene, acetone, chloroform	Soluble in ether, alcohol, benzene, acetone, chloroform	Weast 1983
Partition coefficients:			
Log K_{ow}	1.86	2.09 (recommended value); 2.06	NLM 2022a, 2022b
Log K_{oc}	1.69 (estimated)	1.56 (estimated)	NLM 2022a, 2022b
Vapor pressure	200 mmHg at 25°C	265 mmHg at 20°C 395 mmHg; 410 mmHg at 30°C	Stevens 1979; NLM 2022a, 2022b
Henry's law constant at 24.8°C	$4.86x10^{-3}$ atm-m^3/mol	$8.30x10^{-3}$ atm-m^3/mol	ATSDR 2022b
Autoignition temperature	460°C	460°C	NLM 2022a, 2022b
Flashpoint	2°C; 6°C;	2°C	NLM 2022a, 2022b
Flammability limits	Class IB Flammable Liquid: flash point <73°F and boiling point ≥ 100°F	Class IB Flammable Liquid: flash point <73°F and boiling point ≥ 100°F	NLM 2022a, 2022b
Conversion factors in air at 25°C	1 ppm (v/v)=3.96 mg/m^3 1 mg/m^3=0.25 ppm (v/v)	1 ppm (v/v)=3.96 mg/m^3 1 mg/m^3=0.25 ppm (v/v)	
Explosive limits	5.6–12.8% in air	9.7–12.8% in air	NLM 2022a, 2022b