

## CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

### 4.1 CHEMICAL IDENTITY

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

1,2-Dichloroethene is also known as 1, 2-dichloroethylene, acetylene dichloride, and 1,2-DCE. The substance is a highly flammable, colorless liquid with a discernable odor (NLM 2022a, 2022b).

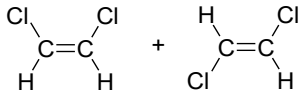
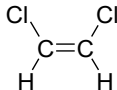
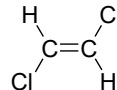
### 4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of 1,2-dichloroethene is presented 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 halogenated VOCs and both have vapor densities heavier than air (NLM 2022a, 2022b).

Both isomers have high vapor pressure and Henry's law constants and have been described as soluble in most organic solvents such as alcohol and ether (NLM 2022a, 2022b).

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

Characteristic	Information <sup>a</sup>		
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 <sup>b</sup>	(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 <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>
SMILES	C1C=CCl	C1C=CCl	C1C=CCl
Chemical structure			
CAS Registry Number	540-59-0	156-59-2	156-60-5

<sup>a</sup>All information from NLM (2022a; cis-1,2-dichloroethene) and NLM (2022b; trans-1,2-dichloroethene), except where noted.

<sup>b</sup>Bennett 1981.

CAS = Chemical Abstracts Services

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**Table 4-2. Physical and Chemical Properties of cis- and trans-1,2-Dichloroethene<sup>a</sup>**

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 <sup>3</sup> )	1.2837	1.2565	NLM 2022a, 2022b
Odor	Slightly acrid, chloroform-like odor	Slightly acrid, chloroform-like odor	NLM 2022a, 2022b
Odor threshold:			
Water	No data	No data	
Air	No data	Odor low: 0.3357 mg/m <sup>3</sup> ; odor high 1,975.00 ppm	NLM 2022b
Taste threshold	No data	No data	
Solubility:			
Water (at 25°C)	6,410 mg/L at 25°C	4,520 mg/L at 25°C	NLM 2022b
Organic solvents	Soluble in ether, alcohol, benzene, acetone, chloroform	Soluble in ether, alcohol, benzene, acetone, chloroform	Weast 1983
Partition coefficients:			
Log K <sub>ow</sub>	1.86	2.09 (recommended value); 2.06	NLM 2022a, 2022b
Log K <sub>oc</sub>	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 <sup>-3</sup> atm-m <sup>3</sup> /mol	8.30x10 <sup>-3</sup> atm-m <sup>3</sup> /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

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**Table 4-2. Physical and Chemical Properties of cis- and trans-1,2-Dichloroethene<sup>a</sup>**

Conversion factors in air at 25°C	1 ppm (v/v)=3.96 mg/m <sup>3</sup> 1 mg/m <sup>3</sup> =0.25 ppm (v/v)	1 ppm (v/v)=3.96 mg/m <sup>3</sup> 1 mg/m <sup>3</sup> =0.25 ppm (v/v)	
Explosive limits	5.6–12.8% in air	9.7–12.8% in air	NLM 2022a, 2022b

<sup>a</sup>All information from NLM (2022a; cis-1,2-dichloroethene) and NLM (2022b; trans-1,2-dichloroethene), except where noted.