

## CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

### 4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of chloroform is presented in Table 4-1.

Table 4-1. Chemical Identity of Chloroform		
Characteristic	Information	Reference
Chemical name	Chloroform, trichloromethane	NLM 2023
Synonym(s) and registered trade name(s)	Chloroform, methenyl trichloride, methane trichloride, methyl trichloride, Freon 20, R 20, R 20 refrigerant	
Chemical formula	CHCl <sub>3</sub>	
SMILES	C(Cl)(Cl)Cl	
Chemical structure	$\begin{array}{c} \text{Cl} \\   \\ \text{H}-\text{C}-\text{Cl} \\   \\ \text{Cl} \end{array}$	
CAS Registry Number	67-66-3	

CAS = Chemical Abstracts Service; SMILES = Simplified Molecular Input Line Entry System

### 4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of chloroform is presented in Table 4-2.

## 4. CHEMICAL AND PHYSICAL INFORMATION

**Table 4-2. Physical and Chemical Properties of Chloroform**

Property	Information	Reference
Molecular weight	119.37 g/mol	NLM 2023
Color	Colorless	NLM 2023
Physical state	Liquid	NLM 2023
Melting point	-63.2°C -63.47°C	NLM 2023
Boiling point	61.12°C	NLM 2023
Density at 20°C	1.484 g/cm <sup>3</sup>	NLM 2023
Density at 25°C	1.4832 g/cm <sup>3</sup> 1.4778 g/cm <sup>3</sup>	
Vapor density (air = 1)	4.12	NLM 2023
Odor	Pleasant, ethereal, nonirritating, sweet	NLM 2023
Odor threshold:		
Water	2.4 ppm (w/v)	NLM 2023
Air	51–307 ppm (w/v)	NLM 2023
Solubility:		
Water at 25°C	7,950 mg/L	NLM 2023
Organic solvents	Miscible with principal organic solvents, alcohol, benzene, ether, petroleum ether, carbon tetrachloride, carbon disulfide, oils	NLM 2023
Partition coefficients:		
Log K <sub>ow</sub>	1.97	NLM 2023
Log K <sub>oc</sub>	1.5–2.29	NLM 2023
Vapor pressure:		
at 20°C	159 mm Hg	Boublik et al. 1984
at 25°C	197 mm Hg	NLM 2023
Henry's law constant:		
at 20°C	3.00x10 <sup>-3</sup> atm·m <sup>3</sup> /mol	Nicholson et al. 1984
at 24.8°C	3.67x10 <sup>-3</sup> atm·m <sup>3</sup> /mol	Gossett 1987; NLM 2023
Autoignition temperature	>1,000°C Not flammable	Deshon 1979 NLM 2023
Flashpoint	None	Deshon 1979
Flammability limits	No data	
Conversion factors <sup>a</sup>	1 ppm (v/v)=4.95 mg/m <sup>3</sup> 1 mg/m <sup>3</sup> =0.20 ppm (v/w)	
Explosive limits	No data	

<sup>a</sup>An atmospheric pressure of 1 atm is assumed and a temperature of 20°C.