CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

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

Table 4-1. Chemical Identity of Carbon Disulfide

Characteristic	Information	Reference
Chemical name	Carbon disulfide	NLM 2023
Synonym(s) and registered trade name(s)	Carbon bisulphide; carbon disulphide; carbon sulfide; carbon sulphide; dithiocarbonic anhydride; sulphocarbonic anhydride; Weeviltox®; Caswell No. 162®	NLM 2023
Chemical formula	CS_2	NLM 2023
SMILES	C(=S)=S	NLM 2023
Chemical structure	S=C=S	NLM 2023
CAS Registry Number	75-15-0	NLM 2023

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 carbon disulfide is presented in Table 4-2.

Table 4-2. Physical and Chemical Properties of Carbon Disulfide

Property	Information	Reference
Molecular weight	76.15 g/mol	NLM 2023
Color	Clear, colorless, or faintly yellow	Sax and Lewis 1987
Physical state	Highly refractive, mobile liquid	Windholz 1983
Melting point	-110.8°C -111.7°C	Weast 1989 NLM 2023
Boiling point	46.5°C (at 760 torr)	Windholz 1983
Density at 15°C at 20°C at 30°C	 1.27055 g/mL 1.2632 g/mL 1.24817 g/mL	 Windholz 1983 Windholz 1983 Windholz 1983
Odor	Purest distillates have sweet, pleasing, and ethereal odor; commercial and reagent grades have foul sulfuric “rotten egg” smell	ATSDR 1999; Flick 1985; Windholz 1983

Table 4-2. Physical and Chemical Properties of Carbon Disulfide

Odor threshold:		
Water	0.0026 mg/L (faint odor)	Verschueren 1983
Air	0.31–0.65 mg/m^3 (0.1–0.2 ppm)	ACGIH 1986
	Low=0.0243 mg/m^3 (0.008 ppm)	Ruth 1986
	High=23.1 mg/m^3 (7.39 ppm)	Ruth 1986
	0.31 mg/m^3 (0.1 ppm) (response in 50% of subjects)	MCA 1968
	0.65 mg/m^3 (0.21 ppm) (response in 100% of subjects)	MCA 1968
	0.05 mg/m^3 (0.016 ppm) (perception in humans)	Verschueren 1983
	0.04 mg/m^3 (0.01 ppm) (nonperception with adverse reflex response in humans)	Verschueren 1983
Taste threshold	No data	
Solubility:		
Water		
at 20°C	2,940 mg/L	Windholz 1983
at 22°C	2,300 mg/L	Verschueren 1983
Organic solvents	Miscible with anhydrous methanol, ethanol, ether, benzene, chloroform, carbon tetrachloride, and oils	Windholz 1983
Partition coefficients:		
Log K_{ow}	1.84–2.16 (calculated)	Verschueren 1983
Log K_{oc}	1.68	NLM 2023
Vapor pressure		
at 0°C	127.0 mmHg	Flick 1985
at 10°C	200 mmHg	Verschueren 1983
at 20°C	260 mmHg	Verschueren 1983
at 20°C	297.5 mmHg	Timmerman 1978
at 25°C	353.6 mmHg	Worthing 1987
at 30°C	430 mmHg	Verschueren 1983
Henry's law constant at 25°C	1.33x10^{-2} atm m^3/mol	EPA 1981a
Autoignition temperature	100°C	Windholz 1983; Sax and Lewis 1987
	125–135°C	Worthing 1987
Flashpoint	-30°C (closed cup)	NFPA 1986; Sax and Lewis 1987; Windholz 1983
Flammability limits in air	1–50% (v/v) (explosive range)	Flick 1985; Windholz 1983
	1.3–50%	NFPA 1986; OSHA 2022
Conversion factors	0.32 ppm=1 mg/m^3	Beauchamp et al. 1983
Explosive limits	Lower=1%	NLM 2023
	Upper=50%	

Carbon disulfide is a volatile mobile liquid. It is soluble in water and miscible with several organic solvents. If released to the environment, it is expected to possess high mobility in soil given its low soil adsorption coefficient, which could result in its leaching into groundwater; however, its high volatility is

likely to reduce its movement into groundwater. The large Henry's Law constant suggests that if released to surface waters it will volatilize rapidly. The low log K_{ow} indicates that it is not likely to bioconcentrate in aquatic organisms.