3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

The chemical identity of carbon disulfide is located in Table 3-l.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

The physical and chemical properties of carbon disulfide are located in Table 3-2.

TABLE 3-1. Chemical Identity of Carbon Disulfide

Characteristic	Information	Reference
Chemical name	Carbon disulfide	HSDB 1995
Synonym(s)	Carbon bisulphide; carbon disulphide; carbon sulfide; carbon sulphide; dithiocarbonic anhydride; sulphocarbonic anhydride	HSDB 1995
Registered trade name(s)	Weeviltox® Caswell No. 162®	HSDB 1995 HSDB 1995
Chemical formula	CS_2	
Chemical structure	S=C=S	
Identification numbers:		
CAS registry	75-15-0	HSDB 1995
NIOSH RTECS	FF6650000	HSDB 1995
EPA hazardous waste	P022 (pure) F-005 (as a mixture component)	HSDB 1995
OHM/TADS	7216633	HSDB 1995
DOT/UN/NA/IMCO shipping	UN 1131; IMCO 6.1	HSDB 1995
HSDB	52	HSDB 1995
NCI	C04591	HSDB 1995

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/ Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

TABLE 3-2. Physical and Chemical Properties of Carbon Disulfide

Property	Information	Reference
Molecular weight	76.14	Windholz 1983
Color	Clear, colorless, or faintly yellow	Sax and Lewis 1987
	Colorless	Windholz 1983
Physical state	Highly refractive, mobile liquid	Windholz 1983
Melting point	-110.8°C	Weast 1989
	-111.5°C	HSDB 1995
Boiling point	46.5°C (at 760 torr)	Windholz 1983
Density		
at 15°C	1.27055 g/mL	Windholz 1983
at 20°C	1.2632 g/mL	Windholz 1983
at 30°C	1.2481 g/mL	Windholz 1983
Odor	Purest distillates have sweet, pleasing, and ethereal odor; commercial and reagent grades are foul smelling	Flick 1985; Windholz 1983
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 (0.2 ppm) (response in 100% of subjects)	MCA 1968
	0.05 mg/m^3 (0.02 ppm) (perception in humans)	Verschueren 1983
	0.04 mg/m^3 (0.01 ppm) (nonperception with adverse reflex response in humans)	Verschueren 1983
Solubility:		
Water		
at 20°C	2940 mg/L	Windholz 1983
at 22°C	2300 mg/L	Verschueren 1983
Organic solvents	Miscible with anhydrous methanol, ethanol, ether, benzene, chloroform, carbon tetrachloride, and oils	Windholz 1983

TABLE 3-2. Physical and Chemical Properties of Carbon Disulfide (*continued*)

Property	Information	Reference
Partition coefficients:		
Log K_{ow}	1.84–2.16 (calculated)	Verschueren 1978
Log K_{oc}	1.80	HSDB 1995
Vapor pressure		
at 10°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	352.6 mmHg	Worthing 1987
at 30°C	430 mmHg	Verschueren 1983
Henry's law constant	$1.22x10^{-2}$ atm m^3/mol	EPA 1981
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)[a] (explosive range)	Flick 1985; Windholz 1983
	1.3–50%	NFPA 1986; Weiss 1980
Conversion factors	0.32 ppm = 1 mg/m^3	Beauchamp et al. 1983
Explosive limits	lower = 1% upper = 50%	OHMTADS 1995

[a]v/v = percent "volume in volume," which expresses the number of milliliters of pure analyte vapor in 100 milliliters of air mixture (ACGIH 1995)