3. CHEMICAL AND PHYSICAL INFORMATION

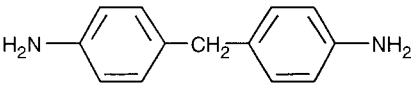
3.1 CHEMICAL IDENTITY

Methylenedianilines are diphenylmethane compounds with an amino group added to each benzene ring. Depending on the position of the amino group, methylenedianilines can exist in six isomeric forms: 2,2´-methylenedianiline; 2,3´-methylenedianiline; 2,4´-methylenedianiline; 3,3´-methylenedianiline; 3,4´-methylenedianiline; and 4,4´-methylenedianiline. Of the six isomers, 2,2´-methylenedianiline and 2,4'-methylenedianiline are produced on a small scale as research chemicals (HSDB 1996). The isomer 4,4´-methylenedianiline is produced in the United States for industrial use. Therefore, this profile will limit its discussion to 4,4´-methylenedianiline. Information regarding the chemical identity of 4,4´-methylenedianiline is presented in Table 3-l.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of 4,4´-methylenedianiline is presented in Table 3-2. Exposure of 4,4´-methylenedianiline to air and light results in polymerization and oxidation of the compound, as evidenced by darkening of color and polymerization leading to the formation of polymeric amines (IARC 1986; Moore 1978). When heated to decomposition, 4,4´-methylenedianiline emits toxic fumes of aniline and nitrogen oxides (NIEHS 1994). It is a weak base (pH 7.7, Allied Chemical Corp. 1978), but its experimentally determined pk_a value was not located in the literature. The estimated pk_a for this compound is 4.88 (EPA 1995). Since 4,4´-methylenedianiline is a base, it forms dihydrochloride salts with hydrochloric acid (IARC 1986). The dihydrochloride of 4,4´-methylenedianiline or other salts of the compound with strong inorganic acids will be more water soluble than the free base. The dihydrochloride salt is soluble in water (NIEHS 1994).

Table 3-1. Chemical Identity of 4,4′-Methylenedianiline

Characteristic	Information	Reference
Chemical name	4,4′-Methylenedianiline	
Synonym(s)	4,4′-Methylene-bis(benzeneamine); 4,4′-diaminodiphenylmethane; 4,4′-methylenebisaniline; p,p′-methylenedianiline; MDA; Methylenedianiline	RTECS 1996
Registered trade name(s)	Ancamine TL; Epicure DDM; Tonox Jeffamine AP-20	IARC 1986 RTECS 1996
Chemical formula	$C_{13}H_{14}N_2$	Merck 1989
Chemical structure		Merck 1989
Identification numbers:		
CAS Registry	101-77-9	HSDB 1996
NIOSH RTECS	BY5425000	HSDB 1996
EPA Hazardous Waste	No data	
OHM/TADS	No data	
DOT/UN/NA/IMCO	UN2651	RTECS 1996
HSDB	2541	HSDB 1996
NCI	C54604	HSDB 1996

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; IARC = International Agency for Research on Cancer; 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 4,4′-Methylenedianiline

Property	Information	Reference
Molecular weight	198.27	Lide 1994
Color	Colorless to pale yellow or light brown	IARC 1986; Lewis 1993
Physical state	Crystalline solid	Moore 1978
Melting point	92–3 °C	Lide 1994
Boiling point	398–9 °C	Lide 1994
Specific gravity	1.1	IARC 1986
Odor	Faint amine-like	Moore 1978
Odor threshold:		
Water	No data	
Air	No data	
Solubility:		
Water at 25 °C	1,000 mg/L; slightly soluble	Moore 1978; Merck 1989
Organic solvent(s)	Very soluble in ethanol, benzene and diethyl ether	Merck 1989; Lide 1994
Partition coefficients:		
Log K_{ow}	1.59	HSDB 1996
Log K_{oc}	2.24 (estimated)	Lyman 1990
Vapor pressure:		
at 25 °C	2.15×10^{-7} mm Hg (estimated from H and water solubility)	Thomas 1990
at 197 °C	1 mm Hg	IARC 1986
Henry's law constant (H) at 25 °C	5.6×10^{-11} atm-m^3/mole (estimated)	HSDB 1996
Autoignition temperature	No data	
Flashpoint	221.1 °C (closed cup); 220 °C (closed cup)	Moore 1978; NFPA 1994
Flammability limits at 25 °C	No data	
NFPA Hazard Class:		NFPA 1994
Health	3 (material extremely hazardous to health)	
Flammability	1 (material must be preheated before ignition)	
Reactivity	0 (material normally stable even under fire conditions and is not reactive with water)	
Conversion factors (25 °C)	1 mg/m^3 = 8.11 ppm 1 ppm = 0.123 mg/m^3	IARC 1986
Explosive limits	No data	

NFPA = National Fire Protection Association