CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Data pertaining to the chemical identity of NDMA are listed in Table 4-1.

Table 4-1. Chemical Identity of N-Nitrosodimethylamine

Characteristic	Information	Reference
Chemical name	Methanamine, N-methyl-N-nitroso	O'Neil 2013
Synonym(s) and registered trade name(s)	N-Nitrosodimethylamine; dimethylnitrosamine; DMNA; DMN; NDMA	O'Neil 2013
Chemical formula	$C_2H_6N_2O$	O'Neil 2013
Chemical structure	$(CH_3)_2N–N=O$	O'Neil 2013
CAS Registry Number	62-75-9	O'Neil 2013

CAS = Chemical Abstracts Service

4.2 PHYSICAL AND CHEMICAL PROPERTIES

The physical and chemical properties of NDMA are presented in Table 4-2.

Table 4-2. Physical and Chemical Properties of N-Nitrosodimethylamine

Property	Information	Reference
Molecular weight	74.08	Weast 1983
Color	Yellow	IARC 1978
Physical state	Liquid	IARC 1978
Melting point	-25°C	Lyman 1985
Boiling point	154°C	Weast 1983
Density at 20°C	1.0059 (specific gravity, 20/4°C)	EPA 2014a
Odor	No distinct odor	Frank and Berry 1981
Odor threshold:		
Water	Not available	
Air	Not available	
Solubility:		
Water at 20°C	Miscible	Mirvish et al. 1976
Organic solvents	Soluble in alcohol, ether, other organic solvents	IARC 1978; Weast 1983

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-2. Physical and Chemical Properties of N-Nitrosodimethylamine

Partition coefficients:		
Log K_{ow}	-0.57	Hansch et al. 1995
Log K_{oc}	1.07 (estimated using Equation 4-8)	Lyman 1982
Vapor pressure at 20°C	2.7 mmHg	Klein 1982
Henry's law constant	1.99×10^{-6} atm-m^3/mol at 37°C; 2.63×10^{-7} atm-m^3/mol at 20°C (estimated using vapor pressure and water solubility data); 2.24×10^{-6} atm-m^3/mol at 25°C	Haruta et al. 2011; Mirvish et al. 1976
Autoignition temperature	No data	
Flashpoint	No data	
Flammability limits	No data	
Conversion factors	ppm (v/v)x3.08=mg/m^3 mg/m^{3}x0.325=ppm (v/v)	