

### 3. CHEMICAL AND PHYSICAL INFORMATION

#### 3.1 CHEMICAL IDENTITY

Data pertaining to the chemical identity of NDMA are listed in Table 3-1.

#### 3.2 PHYSICAL AND CHEMICAL PROPERTIES

The physical and chemical properties of NDMA are presented in Table 3-2.

## 3. CHEMICAL AND PHYSICAL INFORMATION

TABLE 3-1. Chemical Identity of N-Nitrosodimethylamine

	Value	Reference
Chemical name	Methanamine, N-methyl-N-nitroso	CAS 1988
Synonyms	N-nitrosodimethylamine; dimethylnitrosamine; DMNA; DMN; NDMA	CAS 1988
Trade name(s)	ND	
Chemical Formula	C2 H6 N2 O	SANSS 1988
Chemical Structure	(CH <sub>3</sub> ) <sub>2</sub> N-N=O	SANSS 1988
Identification Numbers:		
CAS Registry	62-75-9	CAS 1988
NIOSH RTECS	IQ0525000	RTECS 1988
EPA Hazardous Waste	P082	RTECS 1988
OHM-TADS	7217418	OHM-TADS 1988
DOT/UN/NA/IMCO	ND	
HSDB	1667	HSDB 1988
NCI	ND	

ND = No Data

CAS = Chemical Abstract Service

NIOSH = National Institute for Occupational Safety and Health

RTECS = Registry of Toxic Effects of Chemical Substances

EPA = Environmental Protection Agency

OHM-TADS = Oil and Hazardous Materials - Technical Assistance Data Base

DOT/UN/NA/IMCO = Department of Transportation/United Nations/North

America/International Maritime Consultive Organization

HSDB = Hazardous Substances Data Bank

NCI = National Cancer Institute

## 3. CHEMICAL AND PHYSICAL INFORMATION

TABLE 3-2. Physical and Chemical Properties of N-Nitrosodimethylamine

Property	Value	Reference
Molecular weight	74.08	Weast 1983
Color	yellow	IARC 1978
Physical State	liquid	IARC 1978
Melting point	-25°C (estimated) -50°C (estimated)	Lyman 1985 EPA 1986
Boiling point	154°C	Weast 1983
Specific gravity, 20/4°C	1.0059	Weast 1983
Odor	No distinct odor	Frank and Berry 1981
Odor threshold	Not available	
Solubility		
Water	Miscible	Mirvish et al. 1976
Organic solvents	Soluble in alcohol, ether, other organic solvents	Weast 1983, IARC 1978
Partition coefficient		
Log octanol/water	-0.57	Hansch and Leo 1985
Log K <sub>oc</sub>	1.07 (estimated using Equation 4-8)	Lyman 1982
Vapor pressure	2.7 mm Hg (20°C)	Klein 1982
Henry's Law constant		
at 37°C	$1.99 \times 10^{-6}$ atm-m <sup>3</sup> /mol	Mirvish et al. 1976
at 20°C	$2.63 \times 10^{-7}$ atm-m <sup>3</sup> /mol (estimated using vapor pressure and water solubility data)	

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TABLE 3-2 (continued)

Property	Value	Reference
Autoignition temperature, °C	ND	
Flashpoint, open cup	ND	
Flammability limits in air	ND	
Conversion factors		
ppm (v/v) to mg/m <sup>3</sup> in air (20°C)		ppm (v/v) x 3.08 = mg/m <sup>3</sup>
mg/m <sup>3</sup> to ppm (v/v) in air (20°C)		mg/m <sup>3</sup> x 0.325 = ppm (v/v)

ND = no data