

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Data pertaining to the chemical identity of N-nitrosodi-n-propylamine are listed in Table 3-1.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

The physical and chemical properties of N-nitrosodi-n-propylamine are presented in Table 3-2.

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TABLE 3-1. Chemical Identity of N-Nitrosodi-n-Propylamine

	Value	Reference
Chemical name	1-Propanamine, N-nitroso-N-propyl	CAS 1988
Synonyms	N-nitrosodipropylamine; N,N-dipropylnitrosamine; N-Nitroso-N-di-n-propylamine; NDPA; DPNA; DPN	SANSS 1988; HSDB 1988
Trade name(s)	Not available	
Chemical formula	C ₆ H ₁₄ N ₂ O	CAS 1988
Chemical structure	$ \begin{array}{c} \text{CH}_3\text{-CH}_2\text{-CH}_2 \\ \quad \quad \quad \backslash \\ \quad \quad \quad \text{N-N=O} \\ \quad \quad \quad / \\ \text{CH}_3\text{-CH}_2\text{-CH}_2 \end{array} $	SANSS 1988
Identification numbers:		
CAS Registry	621-64-7	CAS 1988
NIOSH RTECS	JL9700000	RTECS 1988
EPA Hazardous Waste	U111	RTECS 1988
OHM-TADS	8300201	OHM-TADS 1988
DOT/UN/NA/IMCO	Not available	
HSDB	5108	HSDB 1988
NCI	Not available	

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

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TABLE 3-2. Chemical and Physical Properties of
N-Nitrosodi-n-Propylamine

Property	Value	Reference
Molecular weight	130.19	Weast 1983
Color	Yellow	IARC 1978
Physical state	Liquid	IARC 1978
Melting point	6.6°C (estimated) -12°C (estimated)	Lyman 1985 EPA 1986a
Boiling point	206°C	Weast 1983
Specific gravity, 20/4°C	0.9163	Weast 1983
Odor	Not available	
Odor threshold		
Water	Not available	
Air	Not available	
Solubility		
Water	9,894 mg/L (23-25°C)	Mirvish et al. 1976
Organic solvents	Soluble in alcohol, ether, other organic solvents	Weast 1983; IARC 1978
Partition coefficient		
Log octanol/water	1.36	Hansch and Leo 1985
Log K _{oc}	2.11 (estimated)	
Vapor pressure	0.086 mm Hg (20°C) (estimated)	Klein 1982
Henry's Law constant	1.47x10 ⁻⁶ atm-m ³ /mole at 20°C (estimated from vapor pressure and water solubility data)	
Autoignition temperature	Not available	

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TABLE 3-2 (continued)

Property	Value	Reference
Flashpoint	Not available	
Flammability limits in air	Not available ^a	
Conversion factors		
ppm (v/v) to mg/m ³ in air (20°C)	ppm (v/v) x 5.41 = mg/m ³	
mg/m ³ to ppm (v/v) in air (20°C)	mg/m ³ x 0.185 = ppm (v/v)	

^aVapor probably does not form an explosive mixture with air at ordinary temperatures (OHM-TADS 1988).