

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Information regarding the chemical identity of 2,4- and 2,6-DNT is located in Table 3-1.

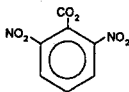
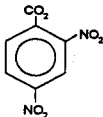
3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of 2,4- and 2,6-DNT is located in Table 3-2.

Data regarding specific isomers of DNT have been provided whenever possible. However, DNT is generally produced as a technical-grade mixture of the two isomers, with approximately 5% other substances. This 5% contains predominantly the other isomers of DNT, which are not discussed in this profile. Where information pertains to Tg-DNT, it has been so noted.

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TABLE 3-1. Chemical Identity of 2,4- and 2,6-Dinitrotoluene

Characteristic	Information	Information	Reference
Chemical Name	2,4-Dinitrotoluene	2,6-Dinitrotoluene	HSDB 1998
Synonym(s)	1-Methyl-2,4-dinitrobenzene; 2,4-dinitrotoluol; 2,4-DNT	1-Methyl-2,6-dinitro- benzene; 2,6-DNT	HSDB 1998
Registered trade name(s)	No data	No data	
Chemical formula	$C_7H_6N_2O_4$	$C_7H_6N_2O_4$	HSDB 1998
Chemical structure			
Identification numbers:			
CAS registry	121-14-2	606-20-2	HSDB 1998
NIOSH RTECS	XT1575000	XT1925000	
EPA hazardous waste	U105	U106	HSDB 1998
OHM/TADS	7800118	8300219	HSDB 1998
DOT/UN/NA/IMCO shipping	IMO 6.1 UN 1600 (molten) UN 2038 (solid or liquid)	6.1 UN 1600 (molten) UN 2038 (solid or liquid)	HSDB 1998
HSDB	1144	2931	HSDB 1998
NCI	NCI-C01865	No data	HSDB 1998

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 Chemicals Substances

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TABLE 3-2. Physical and Chemical Properties of 2,4- and 2,6-Dinitrotoluene

Property	Information	Information	Reference
Chemical name	2,4-Dinitrotoluene	2,6-Dinitrotoluene	Lide 1993
Molecular weight	182.14	182.14	HSDB 1998
Color	Yellow	Yellow to red	HSDB 1998
Physical state	Solid	Solid	HSDB 1998
Melting point	71°C	66°C	HSDB 1998
Boiling point	300°C (slight decomposition)	285°C	HSDB 1998
Density	1.3208 (71°C)	1.2833 (111°C)	HSDB 1998
Odor	Slight	Slight	HSDB 1998
Odor threshold:			
Water	No data	No data	HSDB 1998
Air	No data	No data	HSDB 1998
Solubility:			
Water, mg/L	0.03g/100g (22°C)	180 (20°C)	HSDB 1998, Mabey et al. 1982
Organic solvents	Soluble in acetone, alcohol, benzene, ethanol, diethyl ether, pyridine, CS ₂	Soluble in alcohol	Lide 1993
Partition coefficients:			
Log K _{ow}	1.98	1.72 (estimated)	HSDB 1998
Log K _{oc}			
Vapor pressure, torr 25°C	1.4 × 10 ⁻⁴	5.67 × 10 ⁻⁴	HSDB 1998
Henry's law constant: atm-cu m/mol	8.79 × 10 ⁻⁸	9.26 × 10 ⁻⁸	HSDB 1998
Autoignition temperature,	No data	No data	HSDB 1998
Flashpoint, CC	404°F	404°F	HSDB 1998
Flammability limits	No data	No data	HSDB 1998
Conversion factors			
ppm (v/v) to mg/m ³ in air (20°C)	1 ppm = 7.40 mg/m ³	1 ppm = 7.40 mg/m ³	HSDB 1998
mg/m ³ to ppm (v/v) in air (20°C)	1 mg/m ³ = 0.13 ppm	1 mg/m ³ = 0.13 ppm	HSDB 1998

