4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of the individual isomers of DNT is located in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of the individual isomers of DNT is located in Table 4-2. Data regarding specific isomers of DNT have been provided whenever possible. The isomers of DNT have many similar traits, including identical molecular weights, but also have distinguishable qualities. For instance, 2,4-DNT has higher melting and boiling points and a greater solubility in water than 2,6-DNT (HSDB 2012).

DNTs are generally produced as a technical-grade mixture, which consists of approximately 76.5% 2,4-DNT and 18.8% 2,6-DNT. The remaining ~5% consists of other isomers of DNT and minor contaminants such as TNT and the mononitrotoluenes (HSDB 2012). Unspecified forms of DNT (DNT not otherwise specified or NOS) can be characterized under the CAS Registry Number of 25321-14-6. Where information pertains to Tg-DNT or DNT NOS, it has been so noted.

Table 4-1. Chemical Identity of Dinitrotoluenes

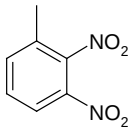
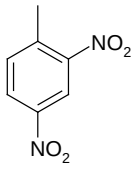
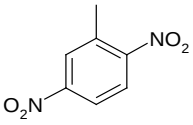
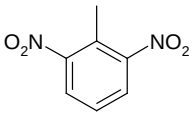
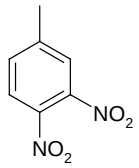
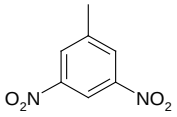
Characteristic	Information[a]		
Chemical name	2,3-Dinitrotoluene	2,4-Dinitrotoluene	2,5-Dinitrotoluene
Synonym(s)	1-Methyl-2,3-dinitrobenzene; 2,3-DNT	1-Methyl-2,4-dinitrobenzene; 2,4-dinitrotoluol; 2,4-DNT	2-Methyl-1,4-dinitrobenzene; 2,5-DNT
Registered trade name(s)	No data	No data	No data
Chemical formula	$C_7H_6N_2O_4$	$C_7H_6N_2O_4$	$C_7H_6N_2O_4$
Chemical structure			
Identification numbers:			
CAS registry	602-01-7	121-14-2	619-15-8
NIOSH RTECS	XT1400000	XT1575000	XT1750000
EPA hazardous waste	No data	U105	No data
OHM/TADS		7800118	
DOT/UN/NA/IMDG shipping	IMO 6.1 UN 1600 (molten) UN 2038 (solid or liquid)	IMO 6.1 UN 1600 (molten) UN 2038 (solid or liquid)	IMO 6.1 UN 1600 (molten) UN 2038 (solid or liquid)
HSDB	5499	1144	5504
NCI	No data	NCI-C01865	No data

Table 4-1. Chemical Identity of Dinitrotoluenes

Characteristic	Information[a]		
Chemical name	2,6-Dinitrotoluene	3,4-Dinitrotoluene	3,5-Dinitrotoluene
Synonym(s)	1-Methyl-2,6-dinitrotoluene; 2,6-DNT	4-Methyl-1,2-Dinitrobenzene; 3,4-DNT	1-methyl-3,5-dinitrobenzene; 3,5-DNT
Registered trade name(s)	No data	No data	No data
Chemical formula	$C_7H_6N_2O_4$	$C_7H_6N_2O_4$	$C_7H_6N_2O_4$
Chemical structure			
Identification numbers:			
CAS registry	606-20-2	610-39-9	618-85-9
NIOSH RTECS	XT1925000	XT2100000	XT2150000
EPA hazardous waste	U106	No data	No data
OHM/TADS	8300219		
DOT/UN/NA/IMDG shipping	IMO 6.1 UN 1600 (molten) UN 2038 (solid or liquid)	IMO 6.1 UN 1600 (molten) UN 2038 (solid or liquid)	IMO 6.1 UN 1600 (molten) UN 2038 (solid or liquid)
HSDB	2931	5501	6463
NCI	No data	No data	No data

[a]All information obtained from HSDB 2012

CAS = Chemical Abstracts Service; DOT/UN/NA/IMDG = 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 Chemical Substances

Table 4-2. Physical and Chemical Properties of Dinitrotoluenes

Property	Information[a]		
Chemical name	2,3-Dinitrotoluene	2,4-Dinitrotoluene	2,5-Dinitrotoluene
Molecular weight	182.14	182.14	182.14
Color	Yellow	Yellow	No data
Physical state	Solid	Solid	Solid
Melting point	59–61 °C	71 °C	52.5 °C
Boiling point	284 °C[b]	300 °C (slight decomposition)	284 °C[b]
Density	No data	1.3208 (71 °C)	1.282 (111 °C)
Odor	No data	Slight	No data
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Solubility:			
Water	220 mg/L (25 °C, estimated)[b]	270 mg/L (22 °C)	220 mg/L (25 °C, estimated)[b]
Organic solvents	No data	Soluble in acetone, alcohol, benzene, ethanol, diethyl ether, pyridine, carbon disulfide	Soluble in ethanol; very soluble in carbon disulfide
Partition coefficients:			
Log K_{ow}	2.18 (estimated)[b]	1.98	2.18 (estimated)[b]
Log K_{oc}	No data	2.56[c]	No data
Vapor pressure at 20 °C	3.97×10^{-4} torr (estimated)[d]	1.4×10^{-4} torr	3.97×10^{-4} torr (estimated)[d]
Henry's law constant at 25 °C			
Autoignition temperature	9.26×10^{-8} atm-m^3/mol (estimated)[b]	5.4×10^{-8} atm-m^3/mol[e]	9.26×10^{-8} atm-m^3/mol (estimated)[b]
Flashpoint			
Flammability limits	No data	No data	No data
Conversion factors	No data	404 °F	404 °F
	No data	No data	No data
Explosive limits	1 ppm=7.40 mg/m^3 1 mg/m^3=0.13 ppm	1 ppm=7.40 mg/m^3 1 mg/m^3=0.13 ppm	1 ppm=7.40 mg/m^3 1 mg/m^3=0.13 ppm

Table 4-2. Physical and Chemical Properties of Dinitrotoluenes

Property	Information[a]		
Chemical name	2,6-Dinitrotoluene	3,4-Dinitrotoluene	3,5-Dinitrotoluene
Molecular weight	182.14	182.14	182.14
Color	Yellow to red	Red	Yellow to red
Physical state	Solid	Solid	Solid
Melting point	66 °C	58.3 °C	93 °C
Boiling point	285 °C	284	315 °C[b]
Density	1.2833 (111 °C)	1.2594 (111 °C)	1.2772 (111 °C)
Odor	Slight	Slight	No data
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Solubility:			
Water	180 mg/L (20 °C)	100 mg/L (25 °C)[f]	145 mg/L (25 °C)
Organic solvents	Soluble in ethanol, chloroform	Soluble in ethanol and carbon disulfide; slightly soluble in chloroform	Soluble in benzene, ethyl ether, ethanol, chloroform, carbon disulfide
Partition coefficients:			
Log K_{ow}	2.10	2.08[g]	2.18 (estimated)[b]
Log K_{oc}	No data	No data	No data
Vapor pressure at 20 °C	5.67×10^{-4} torr	3.97×10^{-4} torr (estimated)[d]	4.05×10^{-4} torr[h]
Henry's law constant at 25 °C			
Autoignition temperature	7.47×10^{-7} atm-m^3/mol (estimated)[b]	9.26×10^{-8} atm-m^3/mol (estimated)[b]	9.26×10^{-8} atm-m^3/mol (estimated)[b]
Flashpoint			
Flammability limits	No data	No data	No data
Conversion factors	404 °F	404 °F	No data
	No data	No data	No data
Explosive limits	1 ppm=7.40 mg/m^3 1 mg/m^3=0.13 ppm	1 ppm=7.40 mg/m^3 1 mg/m^3=0.13 ppm	1 ppm=7.40 mg/m^3 1 mg/m^3=0.13 ppm

[a]All information obtained from HSDB 2012 unless otherwise stated.
[b]EPA 2011
[c]U.S. Army 1980
[d]Neely and Blau 1985
[e]Altschuh et al. 1999
[f]Chemicals Inspection Testing Institute 1992
[g]Nakagawa et al. 1992
[h]AIChE 1992