

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

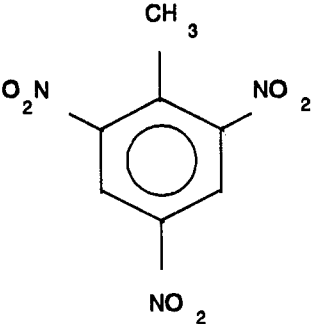
Information regarding the chemical identity of 2,4,6-trinitrotoluene is located in Table 3- 1.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

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

CHEMICAL AND PHYSICAL INFORMATION

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

Characteristic	Information	Reference
Chemical name	2,4,6-Trinitrotoluene	HSDB 1990
Synonym(s)	sym-trinitotoluene; 1-methyl-2,4,6-trinitro- benzene; 2-methyl-1,3,5- trinitrobenzene; alpha- TNT; TNT; alpha-tri- nitrotoluol; tolit; tritol; trotyl oil; trilit	HSDB 1990
Registered trade name(s)	No data	
Chemical formula	$C_7H_5N_3O_6$	Budavari et al. 1989
Chemical structure		Sax and Lewis 1987
Identification numbers:		
CAS registry	118-96-7	Budavari et al. 1989
NIOSH RTECS	XUO175000	HSDB 1990
EPA hazardous waste	No data	
OHM/TADS	7217371	HSDB 1990
DOT/UN/NA/IMCO shipping	TNT, dry or wetted with <30% water (UN 0209/IMO 1.1) TNT, wetted with >30% water (UN 1356/IMO 4.1)	HSDB 1990
HSDB	1146	HSDB 1990
NCI	C56155	HSDB 1990

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 Chemical Substances

CHEMICAL AND PHYSICAL INFORMATION

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

Property	Information	Reference
Molecular weight	227.13	Budavari et al. 1989
Color	Yellow	Budavari et al. 1989
Physical state	Monoclinic needles	Budavari et al. 1989
Melting point	80.1°C	Budavari et al. 1989
Boiling point	240°C (explodes)	HSDB 1990
Specific gravity	1.654	Budavari et al. 1989
Odor	Odorless	NIOSH 1990
Odor Threshold:		
Water	No data	
Air	No data	
Solubility:		
Water at 20°C	130 mg/L	HSDB 1990
Organic solvent(s)	Soluble in acetone and benzene; soluble in alcohol and ether	Budavari et al. 1989
Partition coefficients:		
Log K_{ow}	1.60; 2.2 (measured)–2.7 (estimated)	HSDB 1990; Spanggard et al. 1985
K_{oc}	300 (estimated)–1,100 (measured)	Spanggard et al. 1985
Vapor pressure at 20°C	1.99×10^{-4} mmHg	HSDB 1990
Henry's law constant:		
at 20°C	4.57×10^{-7} atm m ³ /mole	HSDB 1990
at 30°C	No data	HSDB 1994
Autoignition temperature	No data	HSDB 1994
Flashpoint	Explodes	NIOSH 1994
Flammability and Reactivity	4.4	HSDB 1994
Conversion factors	1 ppm = 9.28 mg/m ³ 1 mg/m ³ = 0.108 ppm	NIOSH 1973
Explosive temperature	464°F	HSDB 1994
Explosive limits	No data	NIOSH 1990

