

### **3. CHEMICAL AND PHYSICAL INFORMATION**

#### **3.1 CHEMICAL IDENTITY**

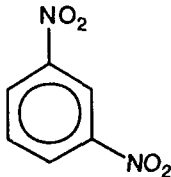
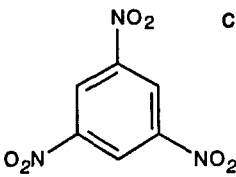
Information regarding the chemical identity of 1,3-DNB and 1,3,5-TNB is located in Table 3-1.

#### **3.2 PHYSICAL AND CHEMICAL PROPERTIES**

Information regarding the physical and chemical properties of 1,3-DNB and 1,3,5-TNB is located in Table 3-2.

## 3. CHEMICAL AND PHYSICAL INFORMATION

TABLE 3-1. Chemical Identity of 1,3-DNB and 1,3,5-TNB

Characteristic	1,3-DNB <sup>a</sup>	1,3,5-TNB <sup>b</sup>
Chemical name	1,3-Dinitrobenzene	1,3,5-Trinitrobenzene
Synonym(s)	m-Dinitrobenzene; 1,3-dinitrobenzol; binitrobenzol; m-DNB; dinitrobenzene	sym-trinitrobenzene; TNB; trinitrobenzene
Registered trade name(s)	No data	No data
Chemical formula	C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> O <sub>4</sub> <sup>c</sup>	C <sub>6</sub> H <sub>3</sub> N <sub>3</sub> O <sub>6</sub> <sup>c</sup>
Chemical structure	 <sup>d</sup>	 <sup>c</sup>
Identification numbers:		
CAS Registry	99-65-0	99-35-4
NIOSH RTECS	CZ7350000	DC3850000
EPA Hazardous Waste	No data	U234
OHM/TADS	7800093 <sup>e</sup>	8400321 <sup>e</sup>
DOT/UN/NA/IMCO	UN1597; IMO 6.1	UN1354; IMO 4.1; UN0214; IMO 1.1
HSDB	4017	6005
NCI	No data	No data

<sup>a</sup>Unless otherwise noted, all references for 1,3-DNB are HSDB 1994

<sup>b</sup>Unless otherwise noted, all references for 1,3,5-TNB are HSDB 1994

<sup>c</sup>Merck 1989

<sup>d</sup>Spanggord *et al.* 1982a

<sup>e</sup>OHM/TADS 1991

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 Substance Data Bank from National Library of Medicine; IARC = International Agency for Research on Cancer; 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; STCC = Standard Transport Commodity Code

## 3. CHEMICAL AND PHYSICAL INFORMATION

TABLE 3-2. Physical and Chemical Properties of 1,3-DNB and 1,3,5-TNB

Property	1,3-DNB <sup>a</sup>	1,3,5-TNB <sup>b</sup>
Molecular weight	168.11 <sup>c</sup>	213.11 <sup>c</sup>
Color	Yellow <sup>d</sup>	Yellow <sup>d</sup>
Physical state	Solid <sup>d</sup>	Solid <sup>d</sup>
Melting point	90 °C <sup>c</sup>	122.5 °C <sup>c</sup>
Boiling point	300–303 °C <sup>c</sup>	315 °C
Density, g/cm <sup>3</sup>	1.575 at 18 °C <sup>c</sup>	1.76 at 20 °C <sup>e</sup>
Odor	No data	No data
Odor threshold:		
Air	No data	No data
Water	No data	No data
Solubility:		
Water at 20 °C	0.5 g/L <sup>e</sup>	3.5 g/L <sup>e</sup>
Organic solvent(s)	Soluble in chloroform, ethyl acetate, benzene, alcohol <sup>e</sup>	Soluble in benzene, methanol, alcohol, ether and carbon disulfide <sup>e</sup>
Partition coefficients:		
Log K <sub>ow</sub>	1.49 <sup>f</sup>	1.18 <sup>f</sup>
Log K <sub>oc</sub>	2.33 <sup>h,i</sup>	1.88 <sup>g,i</sup>
Vapor pressure		
at 20 °C	< 1.0 mm Hg	No data
at 25 °C	No data	3.2x10 <sup>-6</sup> mm Hg <sup>j</sup>
Henry's law constant:		
at 20 °C	2.3x10 <sup>-6</sup> atm-m <sup>3</sup> /mol <sup>k</sup>	No data
at 25 °C	2.33x10 <sup>-6</sup> atm-m <sup>3</sup> /mol	3.08x10 <sup>-9g</sup>
Autoignition temperature	No data	No data
Flashpoint	302 °F	No data
Flammability limits		
at 25 °C	No data	No data
Conversion factors <sup>i</sup>	1 ppm = 6.86 mg/m <sup>3</sup>	1 ppm = 8.70 mg/m <sup>3</sup>
Explosive limits	No data	No data

<sup>a</sup>Unless otherwise noted, all references for 1,3-DNB are HSDB 1994

<sup>b</sup>Unless otherwise noted, all references for 1,3,5-TNB are HSDB 1994

<sup>c</sup>Lide 1990

<sup>d</sup>Sax and Lewis 1987

<sup>e</sup>Merck 1989

<sup>f</sup>Hennion and Coquart 1993; Murray et al. 1993

<sup>g</sup>DeNeer et al. 1987

<sup>h</sup>Army 1987b

<sup>i</sup>Calculated value

<sup>j</sup>Extrapolated value

<sup>k</sup>EPA 1985a

