

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

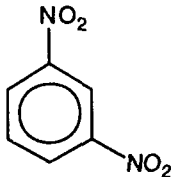
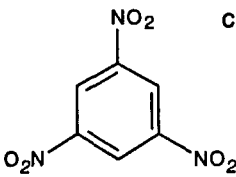
Information regarding the chemical identity of 1,3-DNB and 1,3,5-TNB is located in Table 3-1.

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.

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

Characteristic	1,3-DNB ^a	1,3,5-TNB ^b
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	$C_6H_4N_2O_4^c$	$C_6H_3N_3O_6^c$
Chemical structure	 ^d	 ^c
Identification numbers:		
CAS Registry	99-65-0	99-35-4
NIOSH RTECS	CZ7350000	DC3850000
EPA Hazardous Waste	No data	U234
OHM/TADS	7800093 ^e	8400321 ^e
DOT/UN/NA/IMCO	UN1597; IMO 6.1	UN1354; IMO 4.1; UN0214; IMO 1.1
HSDB	4017	6005
NCI	No data	No data

^aUnless otherwise noted, all references for 1,3-DNB are HSDB 1994

^bUnless otherwise noted, all references for 1,3,5-TNB are HSDB 1994

^cMerck 1989

^dSpanggord *et al.* 1982a

^eOHM/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

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

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

^aUnless otherwise noted, all references for 1,3-DNB are HSDB 1994

^bUnless otherwise noted, all references for 1,3,5-TNB are HSDB 1994

^cLide 1990

^dSax and Lewis 1987

^eMerck 1989

^fHennion and Coquart 1993; Murray et al. 1993

^gDeNeer et al. 1987

^hArmy 1987b

ⁱCalculated value

^jExtrapolated value

^kEPA 1985a

