## 3. CHEMICAL AND PHYSICAL INFORMATION

### 3.1 CHEMICAL IDENTITY

Information regarding the chemical identity of Otto Fuel II and its components is located in Table 3-1.

# 3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of Otto Fuel II and its components is located in Table 3-2.

# TABLE 3-1. Chemical Identity of Otto Fuel II and Its Components<sup>a</sup>

Characteristic	Otto fuel II	Propylene glycol dinitrate	<sup>b</sup> 2-Nitrodiphenylamine <sup>c</sup>	Dibutyl sebacate
Synonym(s)	No data	PGDN; 1,2-propylene glyco dinitrate; 1,2-propanediol, dinitrate; propylene dinitrate isopropylene nitrate; methylnitroglycol; propylene	phenyl; <u>o</u> -nitro-N-phenylaniline; <u>o</u> - ; nitro-diphenylamine <sup>b</sup>	Bis ( <u>n</u> -butyl) sebacate; butyl sebacate; decanedioic acid, dibutyl ester; sebacic acid, dibutyl ester; dibutyl decanedioate; di- <u>n</u> - butylsebacate <sup>a</sup> ; dibutylester kyseliny
Registered trade name(s)	No data	No data	Sudan yellow 1339;    C.I. 10335 <sup>b</sup>	Kodaflex DBS; Staflex DBS; PX 404; Monoplex DBS; Polycizer DBS <sup>f</sup>
Chemical formula	Not applicable	C₃H <sub>6</sub> N₂O <sub>6</sub> <sup>9</sup>	C <sub>12</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> <sup>b</sup>	C <sub>18</sub> H <sub>34</sub> O <sub>4</sub> <sup>†</sup>
Chemical structure	Not applicable	NO2OCH2CHONO2   CH3 C	NO <sub>2</sub> b	0 h <sup>  </sup> CH₃CH₂CH₂CH₂CH₂-O-C-CH₂CH₂CH₂CH₂ CH₃CH₂CH₂CH₂CH₂-O-C-CH₂CH₂CH₂CH₂ <sup>  </sup> O
Identification numbers:				
CAS registry	106602-80-6	6423-43-4 <sup>i</sup>	119-75-5 <sup>b</sup>	109-43-3
NIOSH RTECS	No data	TY 6300000 <sup>h</sup>	No data	VS 1150000
EPA hazardous waste	No data	No data	No data	878212204; 878221572; 878221503 <sup>j</sup>
OHM/TADS	No data	No data	No data	No data
DOT/UN/NA/IMCO shipping	No data	No data	No data	No data
HSDB	No data	No data	No data	309
NCI	No data	No data	No data	No data
<sup>a</sup> All information obtained from 1 <sup>b</sup> Forman 1988 <sup>c</sup> Army 1979 <sup>d</sup> NRC 1982	HSDB 1994 except	<sup>e</sup> RTECS 1994 <sup>f</sup> Sax and Lewis 1989a	<sup>n</sup> SANSS 1994 Sax and Lewis 1989b Chemlist 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 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 ω

# OTTO FUEL II AND ITS COMPONENTS

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# TABLE 3-2. Physical and Chemical Properties of Otto Fuel II and its Components<sup>a</sup>

37. - 1987 - 19 38. - 1988 - 19

Property	Otto fuel II	Propylene glycol dinitrate	2-Nitrodiphenylamine	Dibutyl sebacate
Molecular weight	No data	166.1 <sup>b</sup>	214.23 <sup>c</sup>	314.52 <sup>d</sup>
Color	Reddish-orange <sup>e</sup>	Colorless <sup>†</sup>	Orange <sup>9</sup>	Ciear <sup>d</sup>
Physical state	Oily liquid <sup>e</sup>	Liquid <sup>f</sup>	Solid (orthorhombic crystals) <sup>c</sup>	Liquid <sup>d</sup>
Melting point	-27.7 °C <sup>h</sup>	-27.7° C <sup>f</sup>	75–76 °C <sup>c</sup>	-10 °C
Boiling point	Decomposes at 121 °C <sup>h</sup>	Decomposes at 121 °C <sup>f</sup> ; 92 °C (10 mmHg) <sup>f</sup>	223 °C (20 mmHg) <sup>c</sup>	180 °C (3 mmHg) <sup>d</sup> ; 344–345 °C (pressure unspecified)
Density	1.232 g/mL (25 °C) <sup>h</sup>	1.232 g/mL (25 °C) <sup>1</sup>	1.366 g/mL <sup>c</sup>	0.936 g/mL (20 °C) <sup>d</sup>
Odor	Distinctive <sup>h</sup>	Disagreeablet	No data	No data
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility: Water Organic solvent(s)	Insoluble <sup>h</sup> Alcohols; benzene carbon tetrachloride; hexane; chloroform; toluene; dibutyl phthalate; acetone; trichloroethylene <sup>h</sup>	0.13 g/100 mL <sup>f</sup> No data	Insoluble <sup>i</sup> Ethanol, 2 g/100 mL (25 °C) <sup>c</sup> ; Methanol, 2.4 g/100 mL (20 °C) <sup>c</sup> ; Acetone, 43.6 g/100 mL (20 °C) <sup>c</sup> ; Benzene, 51.7 g/100 mL (20 °C) <sup>c</sup>	Insoluble Ether
Partition coefficients:				
Log K <sub>ow</sub>	No data	No data	0.49 <sup>c</sup>	No data
Log K <sub>oc</sub>	No data	No data	No data	No data
Vapor pressure	0.0877 mm Hg (25 °C) <sup>h</sup>	0.09844 mm Hg (25 °C) <sup>j</sup>	0.00001 mm Hg (25 °C) <sup>k</sup>	3 mm Hg (180 °C)
Henry's law constant	No data	No data	No data	No data
Autoignition temperature	121 °C <sup>1</sup>	No data	No data	No data
Flashpoint	130 °C <sup>hg</sup>	No data	No data	178 °C
Flammability limits	Monopropeilant <sup>i</sup>	No data	No data	Slight potential when exposed to heat or flame
Conversion factors	No data	1 ppm = 7.14 mg/m <sup>3 m</sup>	No data	No data
Explosive limits	No data	No data	No data	No data
<sup>a</sup> All information obtair <sup>b</sup> Sax and Lewis 1989 <sup>c</sup> Army 1979	ned from HSDB 1994 unless otherwise b	noted <sup>d</sup> Sax and Lewis 19 <sup>e</sup> Forman 1988 <sup>1</sup> ACGIH 1986	89a <sup>9</sup> Dean 1974 <sup>h</sup> Air Force 1985a <sup>i</sup> American Cyanamid 1982	<sup>I</sup> Crater 1929 <sup>K</sup> Baughman and Perenich 198 <sup>I</sup> Rivera 1974