

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

#### **3.1 CHEMICAL IDENTITY**

Information regarding the chemical identity of diethyl phthalate is located in Table 3-1.

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

Information regarding the physical and chemical properties of diethyl phthalate is located in Table 3-2.

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TABLE 3-1. Chemical Identity of Diethyl Phthalate

Characteristic	Information	Reference
Chemical name	Diethyl phthalate	HSDB 1994
Synonym(s)	1,2-Benzenedicarboxylic acid diethyl ester; diethyl <i>o</i> -phthalate; ethyl phthalate; <i>o</i> -benzenedicarboxylic acid diethyl ester; diethyl ester phthalic acid; phthalol; DEP; diethyl- <i>o</i> -phenylenediacetate	EPA 1989; HSDB 1994; OHM/TADS 1991
Registered trade name(s)	Neantine; Palatinol A; Phthalol; Placidol E; Solvanol; Unimoll DA; Anozol; Estol 1550	HSDB 1994
Chemical formula	C <sub>12</sub> H <sub>14</sub> O <sub>4</sub>	HSDB 1994
Chemical structure		
Identification numbers:		
CAS registry	84-66-2	HSDB 1994
NIOSH RTECS	TI1050000	HSDB 1994
EPA hazardous waste	U088	HSDB 1994
OHM/TADS	7217236	HSDB 1994
DOT/UN/NA/IMCO shipping	No data	
HSDB	926	HSDB 1994
NCI	NCI-C60048	HSDB-1994

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

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**TABLE 3-2. Physical and Chemical Properties of Diethyl Phthalate  
(continued)**

Characteristic	Information	Reference
Henry's law constant <sup>a</sup>	$7.8 \times 10^{-7}$ atm m <sup>3</sup> /mol	EPA 1989
Autoignition temperature	457°C	HSDB 1994
Flashpoint	161°C	HSDB 1994
Flammability limits <sup>b</sup>	0.7% at 187°C	HSDB 1994
Conversion factors	9.07 mg/m <sup>3</sup> = 1 ppm	HSDB 1994
Explosive limits	No data	

<sup>a</sup>Temperature not specified<sup>b</sup>Lower flammability limit given; upper limit not available

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TABLE 3-2. Physical and Chemical Properties of Diethyl Phthalate

Characteristic	Information	Reference
Molecular weight	222.23	Anonymous 1988; Autian 1973
Color	Colorless	HSDB 1994
Physical state	Liquid	HSDB 1994
Melting point	-40.5°C	HSDB 1994
Boiling point	295-302°C	Autian 1973; Banerjee et al. 1990; EPA 1989; HSDB 1990; OHM/TADS 1991; Sax and Lewis 1989
Density at 25°C	1.120 g/mL	Anonymous 1985
Odor	Slight aromatic odor	HSDB 1994
Odor threshold:		
Water	No data	
Air	No data	
Solubility:		
Water at 25°C	1,080 mg/L	Howard et al. 1985; HSDB 1994
Organic solvent(s)	Alcohol, ether, acetone, and benzene; vegetable oils; ketones, esters, aromatic hydrocarbons, and aliphatic solvents	HSDB 1994
Partition coefficients:		
Log $K_{ow}$	1.4-3.3	Callahan et al. 1979; Howard et al. 1985; HSDB 1994; Laane et al. 1987; Leyder and Boulanger 1983; Veith et al. 1980
Log $K_{oc}$	2.65	Wolfe et al. 1980b
Vapor pressure:		
at 20°C	$3.45 \times 10^{-4}$ mmHg	Grayson and Fosbraey 1982
at 25°C	$1.65 \times 10^{-3}$ mmHg	Howard et al. 1985; HSDB 1994