4. CHEMICAL AND PHYSICAL INFORMATION

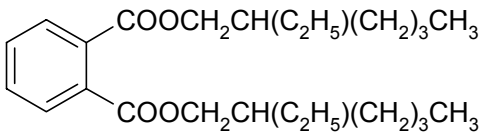
4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of DEHP is located in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of DEHP is located in Table 4-2.

Table 4-1. Chemical Identity of DEHP

Characteristic	Information	Reference
Chemical name	Di(2-ethylhexyl) phthalate	RTECS 2000
Synonym(s)	DEHP; dioctylphthalate; bis(2-ethylhexyl) phathalate	RTECS 2000
Registered trade name(s)	Bisoflex 81; Eviplast 80; Octoil; Plantinol DOP; Staflex DOP	RTECS 2000
Chemical formula	$C_{24}H_{38}O_4$	RTECS 2000
Chemical structure		Howard and Meylan 1997
Identification numbers:		
CAS registry	117-81-7	Cadogan and Howick 1996
NIOSH RTECS	TI0350000	RTECS 2000
EPA hazardous waste	U028	HSDB 1990
OHM/TADS	7216693	HSDB 1990
DOT/UN/NA/IMCO shipping	No data	
HSDB	334	HSDB 1990
NCI	C52733	Montgomery and Welkom 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; NFPA = National Fire Protection Association; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

Table 4-2. Physical and Chemical Properties of DEHP

Property	Information	Reference
Molecular weight	390.57	Howard and Meylan 1997
Color	Colorless	Montgomery and Welkom 1990
Physical state	Liquid	Staples et al. 1997
Melting point	-47 EC	Staples et al. 1997
Boiling point	384 EC	Howard and Meylan 1997
Density	0.984 g/mL at 20 EC	Cadogan and Howick 1996
Odor	Slight odor	HSDB 1990
Odor threshold:		
Water	No data	
Air	No data	
Solubility:		
Water	41 µg/L at 25 EC[a]	Leyder and Boulanger 1983
Organic solvent(s)	Miscible in mineral oil and hexane	HSDB 1990
Partition coefficients:		
Log K_{ow}	7.50	Staples et al. 1997
Log K_{oc}	4.9–6	Staples et al. 1997
Vapor pressure	$1.0x10^{-7}$ mmHg at 25 EC	Staples et al. 1997
Henry's law constant:	$1.71x10^{-5}$ atm-m3/mole at 25 EC	Staples et al. 1997
Autoignition temperature	735 EF (390 EC)	HSDB 1990
Flashpoint	384.8 EF (196 EC) (open cup)	Montgomery and Welkom 1990
Flammability limits	No data	
Conversion factors	1 ppm=15.94 mg/m^3	Clayton and Clayton 1981
Explosive limits	0.3% (lower limit) No data (upper limit)	Montgomery and Welkom 1990

[a]The solubilities of DEHP in distilled water that have been determined both experimentally and theoretically vary between 1.1 and 1,200 µg/L (Staples et al. 1997). The value of 41 µg/L was the lowest experimentally derived value for the solubility of DEHP in distilled water. A value of 3 µg/L for the water solubility of DEHP has been recommended by Staples et al. that is "based on available evidence", rather than any one specific experimentally derived value. Unfortunately, the authors do not indicate how they derived their recommended value of 3 µg/L. Yet, the "true" solubility may be at or below the value of 3 µg/L value, based on estimated solubilities obtained from the SPARC (2.6 µg/L) and EPIWIN (1.1 µg/L) estimation models (Staples et al. 1997). Indeed, in a recent report (Ellington 1996) describing the results obtained from a slow-stir method for determining the water solubility of phthalate esters, the water solubility of a chemical analogue of DEHP, dioctylphthalate (DOP), was found to be 0.51 µg/L. It is likely that the solubility of DEHP in distilled water will be similar to that obtained for DOP using the same experimental method. However, the solubility of DEHP in distilled water has yet to be determined experimentally using the slow-stir method. Thus, it is clear that more experimental data are required before the "true" solubility of DEHP in distilled water can be determined.