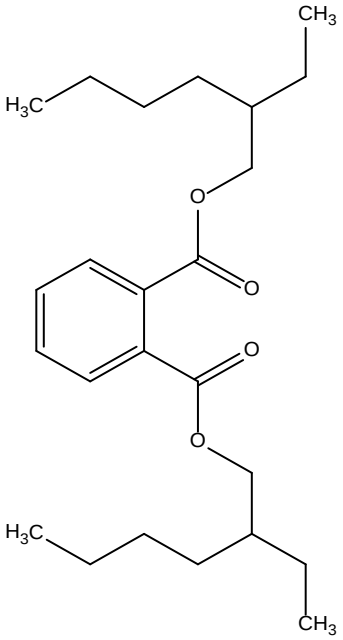
CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Di(2-ethylhexyl)phthalate, also known as DEHP, is an organic ester containing an eight-carbon alcohol moiety widely used as a plasticizer in polymers. DEHP is widely used for a variety of standard products due to its overall performance characteristics, including fusion rate, efficiency, and viscosity (Cadogan and Howick 2001; TURI 2006).

Table 4-1 lists common synonyms, trade names, and other pertinent identification information for DEHP.

Table 4-1. Chemical Identity of DEHP

Characteristic	Information	Reference
Chemical name	Di(2-ethylhexyl)phthalate	RTECS 2013
Synonym(s) and Registered trade name(s)	DEHP; dioctylphthalate; DOP; bis(2-ethylhexyl) phathalate; Bisoflex 81; Eviplast 80; Octoil; Plantinol DOP; Staflex DOP; 1,2-benzenedicarboxylic acid, 1,2-bis(2ethylhexyl) ester	EPA 2012; RTECS 2013
Chemical formula	$C_{24}H_{38}O_4$	RTECS 2013
Chemical structure		Howard and Meylan 1997
CAS Registry Number	117-81-7	RTECS 2013

CAS = Chemical Abstracts Services

4.2 PHYSICAL AND CHEMICAL PROPERTIES

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

Table 4-2. Physical and Chemical Properties of DEHP

Property	Information	Reference
Molecular weight	390.57	Howard and Meylan 1997
Color	Colorless	NIOSH 2016
Physical state	Liquid	Staples et al. 1997
Melting point	-47 °C	Staples et al. 1997
Boiling point	384 °C	Howard and Meylan 1997
Density at 20 °C	0.984 g/cm^3	Cadogan and Howick 2001
Odor	Slight odor	TURI 2006
Odor threshold:	No data	
Solubility:		
Water at 25 °C Water at 20 °C	41 µg/L[a] 1.9 µg/L[a]	Leyder and Boulanger 1983 Letinski et al. 2002
Organic solvents	Miscible in mineral oil; slightly soluble in carbon tetrachloride	Haynes 2014; Larranaga et al. 2016
Partition coefficients:		
Log K_{ow}	7.50	Staples et al. 1997
Log K_{oc}	4.9–6	Staples et al. 1997
Vapor pressure at 25 °C	1.0x10^{-7} mmHg	Staples et al. 1997
Henry's law constant at 25 °C	1.71x10^{-5} atm-m^3/mole	Staples et al. 1997
Autoignition temperature	735 °F (350 °C)	NIOSH 2001
Flashpoint	420 °F (216 °C) (open cup)	NIOSH 2016
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)	NIOSH 2016

[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 highest values are likely to be overestimated as measurements that used the traditional shake flask method often led to these higher values. The value of 41 µg/L was the lowest experimentally derived value for the solubility of DEHP in distilled water. Yet, estimation models, SPARC and EPIWIN, provided solubility estimates of 2.6 and 1.1 µg/L, respectively (Staples et al. 1997), whereas Ellington (1999) found the chemical DEHP analog, dioctylphthalate, to have a solubility of 0.51 µg/L using the slow stir method. Letinski et al. (2002) determined DEHP solubility using the slow stir technique and reported a value of 1.9 µg/L in sterilized well water at 20 °C.