

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Information regarding the chemical identity of di-*n*-octylphthalate is located in Table 3-1.

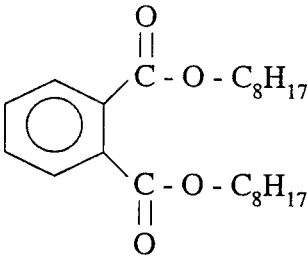
3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the chemical and physical properties of di-*n*-octylphthalate is located in Table 3-2.

There is conflicting information for many of these properties in the literature. A possible explanation for the inconsistencies, as discussed in Chapter 2, may come from the use of the nonspecific term “di-octylphthalate.” This conflict has contributed to significant confusion and misinformation in the literature with respect to di-*n*-octylphthalate and the much more common isomer, di(2-ethylhexyl)phthalate. Although frequently being interpreted as referring to di-*n*-octylphthalate, it is apparent that in almost all cases “di-octylphthalate” and “DOP” have in fact been used as synonyms for di(2-ethylhexyl)phthalate. Therefore, many of the properties found for di-*n*-octylphthalate or di-octylphthalate may possibly be for di(2-ethylhexyl)phthalate.

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TABLE 3-1. Chemical Identity of Di-*n*-octylphthalate

Characteristic	Information	Reference
Chemical name	Di- <i>n</i> -octylphthalate	HSDB 1995
Synonym(s)	1,2-benzenedicarboxylic acid, di- <i>n</i> -octyl ester; 1,2-benzenedicarboxylic acid, dioctyl ester; <i>o</i> -benzenedicarboxylic acid, dioctyl ester; DNOP; DOP; dioctyl 1,2-benzenedicarboxylate; dioctyl <i>o</i> -benzenedicarboxylate; octyl phthalate; dioctyl phthalate; <i>n</i> -octyl phthalate; phthalic acid, dioctyl ester	HSDB 1995; EPA 1987a
Registered trade name(s)	Cellulflux DOP; Dinopol NOP; Polycizer 162; PX-138; Vinicizer 85	HSDB 1995
Chemical formula	C ₂₄ H ₃₈ O ₄	HSDB 1995
Chemical structure		EPA 1987a
Identification numbers:		
CAS registry	117-84-0	HSDB 1995
NIOSH RTECS	TI 1925000	HSDB 1995
EPA hazardous waste	U 107	HSDB 1995
OHM/TADS	8300217	HSDB 1995
DOT/UN/NA/IMCO shipping	No data	
HSDB	1345	IRIS 1995
NCI	No data	

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 Di-*n*-octylphthalate

Property	Information	Reference
Molecular weight	390.54	Clayton and Clayton 1981
	390.56	HSDB 1995
	390.57	EPA 1987b
	390.62	EPA 1987a; Sax and Lewis 1989; NIOSH RTECS 1987
Color	Colorless	EPA 1987a
Physical state	Liquid	EPA 1987a
Melting point	-25°C	EPA 1987a
Boiling point		
at 760 mm Hg	390–420°C	EPA 1993a
at 5 mm Hg	230°C	Sittig 1991
at 4 mm Hg	220–240°C	EPA 1987a
	220°C	HSDB 1995
Density:		
at 25°C	0.978 g/mL	HSDB 1995
Odor	Odorless	EPA 1993
Odor threshold:		
Water	No data	
Air	No data	
Solubility:		
Water at 25°C	0.2 mg/L	EPA 1992a
	3.0 mg/L	Wolfe et al. 1980; HSDB 1995
Organic solvent(s)	Soluble	EPA 1987a
Partition coefficients:		
Log K_{ow}	5.22	EPA 1987a; HSDB 1995
Log K_{oc}	4.28	Wolfe et al. 1980
Vapor pressure at 25°C	1.44×10^{-4} mm Hg	EPA 1987a
Henry's law constant	5.5×10^{-6} H atm-m ³ /mole	EPA 1992a
	6.68×10^{-5} H atm-m ³ /mole	EPA 1992a
Autoignition temperature	No data	
Flashpoint	219°C	Sittig 1991
Flammability limits	No data	
Conversion factors	No data	
Explosive limits	No data	

