

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

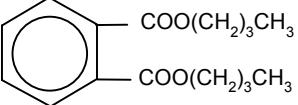
Information regarding the chemical identity of di-*n*-butyl phthalate is located in Table 4-1. Table 4-1 lists common synonyms, trade names, and other pertinent identification information for di-*n*-butyl phthalate.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of di-*n*-butyl phthalate is located in Table 4-2. Table 4-2 lists important physical and chemical properties of di-*n*-butyl phthalate, but is not intended to be all inclusive.

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Table 4-1. Chemical Identity of Di-*n*-butyl Phthalate

Characteristic	Information	Reference
Chemical name	Di- <i>n</i> -butyl phthalate	HSDB 2000
Synonym(s)	1,2-Benzenedicarboxylic acid, dibutyl ester; Butyl phthalate; DBP; Dibutyl- <i>o</i> -phthalate; Dibutyl phthalate; Phthalic acid butyl ester	HSDB 2000; Budavari 1996
Registered trade name(s)	Caswell No. 292; Celluflex DBP; Palatinol C; Polycizer DBP; PX 104; Staflex DBP; Uniflex DB	HSDB 2000
Chemical formula	C ₁₆ H ₂₂ O ₄	Budavari 1996
Chemical structure		Metcalf 1994
Identification numbers:		
CAS Registry	84-74-2	Lewis 1993
NIOSH RTECS	TI0875000	HSDB 2000
EPA Hazardous Waste	U069	EPA 1992
OHM/TADS	7216617	CIS 1999
DOT/UN/NA/IMCO	UN 2810/NA 9095	DOT 1998
HSDB	922	HSDB 2000
NCI	5804	NIH 1999

CAS = Chemical Abstracts Services; CIS = Chemical Information System; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substance 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 4-2. Physical and Chemical Properties of Di-*n*-butyl Phthalate

Property	Information	Reference
Molecular weight	278.34	Budavari 1996
Color	Colorless to faint yellow	HSDB 1999
Physical state	Oily liquid	Lewis 1993
Melting point	-35 EC	Verschueren 1996
Boiling point	340 EC	Budavari 1996
Density at 20 EC	1.04 kg/L	Ashford 1994
Odor	Slight ester-like	EPA 1993
Odor threshold:		
Water	No data	
Air	0.26–1.47 mg/m ³	EPA 1980b
Taste	Strong and bitter taste	HSDB 1999
Solubility:		
Water	11.2 mg/L	Staples et al. 1997
Freshwater at 20 EC	10.1–11.1 mg/L	Shiu et al. 1990
Organic solvent (s)	Very soluble in alcohol, ether, acetone, and benzene	Budavari 1996
Partition coefficients:		
Log K _{ow}	4.72	Hansch et al. 1995
	4.45	Staples et al. 1997
	3.7	de Bruijn et al. 1989
Log K _{oc}	3.14	Russell and McDuffie 1986
	4.17	Sullivan et al. 1982
Vapor pressure at 25 EC	2.01x10 ⁻⁵ mmHg 2.7x10 ⁻⁵ mm Hg	Donovan 1996 Staples et al. 1997
Polymerization	No data	
Photolysis	No data	
Henry's law constant at 25 EC	4.5x10 ⁻⁶ atm-m ³ /mole 8.83x10 ⁻⁷ atm-m ³ /mole	Roy 1994 Staples et al. 1997
Autoignition temperature	403 EC	Weiss 1986
Flashpoint	157 EC	NIOSH 1997
Flammability limits at 25 EC	No data	
Incompatibilities	Reacts explosively with liquid chlorine	Bisesi 1994
Conversion factors (25 EC)	11.36 mg/m ³ =approximately 1 ppm 1 mg/m ³ =0.088 ppm	Bisesi 1994
Explosive limits	Lower explosive limit: 0.5% at 236 EC	NIOSH 1997

HSDB = Hazardous Substance Data Bank; NIOSH = National Institute for Occupational Safety and Health