

## 4. CHEMICAL AND PHYSICAL INFORMATION

### 4.1 CHEMICAL IDENTITY

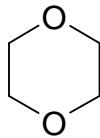
1,4-Dioxane or para-dioxane is also commonly referred to as simply 'dioxane'. However, 1,4-dioxane should not be confused with dioxin (or dioxins), which are a different class of chemical compounds. Information regarding the chemical identity of 1,4-dioxane is located in Table 4-1.

### 4.2 PHYSICAL AND CHEMICAL PROPERTIES

1,4-Dioxane is a colorless volatile liquid. 1,4-Dioxane is also completely miscible in water and organic solvents. The technical-grade product is >99.9% pure, but may contain bis(2-chloroethyl) ether as an impurity (DeRosa et al. 1996). Information regarding the physical and chemical properties of 1,4-dioxane is located in Table 4-2.

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**Table 4-1. Chemical Identity of 1,4-Dioxane**

Characteristic	Information
Chemical name	1,4-Dioxane
Synonym(s)	1,4-diethylenedioxiide; 1,4-dioxacyclohexane; 1,4-dioxanne (French); di(ethylene oxide); diethylene dioxide; diethylene ether; dioksan (Polish); diossano-1,4 (Italian); dioxaan-1,4 (Dutch); dioxan; dioxan-1,4 (German); dioxane; dioxane-1,4; dioxanne (French); dioxyethylene ether; glycol ethylene ether; para-dioxane; <i>p</i> -dioxan (Czech); <i>p</i> -dioxane; <i>p</i> -dioxin, tetrahydro-; tetrahydro-1,4-dioxin; tetrahydro-para-dioxin; tetrahydro- <i>p</i> -dioxin
Registered trade name(s)	No data
Chemical formula	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>
Chemical structure	
Identification numbers:	
CAS Registry	123-91-1
NIOSH RTECS	JG8225000
EPA Hazardous Waste	U108; A toxic waste when a discarded commercial chemical product or manufacturing chemical intermediate or an off-specification commercial chemical product or a manufacturing chemical intermediate
OHM/TADS	No data
DOT/UN/NA/IMDG	UN 1165; IMDG 3.2
HSDB	81
NCI	No data

CAS = Chemical Abstracts Services; CIS = Chemical Information System; DOT/UN/NA/IMDG = 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 1,4-Dioxane**

Property	
Molecular weight (g/mol)	88.11 <sup>a</sup>
Color	Clear <sup>b</sup>
Physical state	Liquid <sup>a</sup>
Melting point	11.8 °C <sup>a</sup>
Boiling point	101.1 °C <sup>a</sup>
Density	1.0329 <sup>a</sup>
Odor	Faint pleasant odor <sup>a</sup>
Odor threshold:	
Water	230 ppm w/v <sup>b</sup>
Air	24 ppm v/v <sup>b</sup>
Taste	No data
Solubility:	
Water	Miscible <sup>c</sup>
Other solvents	Soluble in organic solvents <sup>a</sup>
Partition coefficients:	
Log K <sub>ow</sub>	-0.27 <sup>d</sup>
Log K <sub>oc</sub>	1.23 <sup>b</sup>
Vapor pressure at 25 °C	38.1 mm Hg <sup>e</sup>
OH radical rate constant	1.09x10 <sup>-11</sup> cm <sup>3</sup> /molecule-sec <sup>f</sup>
Henry's law constant at 25 °C	4.80x10 <sup>-6</sup> atm-cm <sup>3</sup> /mole <sup>g</sup>
Autoignition temperature	356 °F (180 °C) <sup>h</sup>
Flashpoint	5–18 °C <sup>a</sup>
Flammability limits at 25 °C	Lower: 2.0%; Upper: 22% <sup>b</sup>
Incompatibilities	Strong oxidizers, decaborane, triethynyl aluminum <sup>h</sup>
Conversion factors (25 °C and 1 atm)	1 ppm = 3.6 mg/m <sup>3</sup> ; 1 mg/m <sup>3</sup> = 0.278 ppm <sup>b</sup>
Explosive limits	Vapor forms explosive mixtures with air over wide range <sup>i</sup>

<sup>a</sup>O'Neil et al. 2001<sup>b</sup>EC 2002<sup>c</sup>Riddick et al. 1986<sup>d</sup>Hansch et al. 1995<sup>e</sup>Daubert and Danner 1985<sup>f</sup>Atkinson 1989<sup>g</sup>Park et al. 1987<sup>h</sup>NIOSH 2001<sup>i</sup>ScienceLab 2005