

## **4. CHEMICAL AND PHYSICAL INFORMATION**

### **4.1 CHEMICAL IDENTITY**

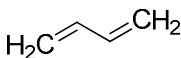
Information regarding the chemical identity of 1,3-butadiene is located in Table 4-1. This information includes synonyms, chemical formula and structure, and identification numbers.

### **4.2 PHYSICAL AND CHEMICAL PROPERTIES**

Information regarding the physical and chemical properties of 1,3-butadiene is located in Table 4-2.

## 4. CHEMICAL AND PHYSICAL INFORMATION

**Table 4-1. Chemical Identity of 1,3-Butadiene<sup>a</sup>**

Characteristic	Information
Chemical name	1,3-Butadiene
Synonyms and trade names	Butadiene; buta-1,3-diene; biethylene; bivinyll; divinyl; vinylethylene; erythrene; alpha,-gamma-butadiene; pyrrolylene <sup>b</sup>
Chemical formula	C <sub>4</sub> H <sub>6</sub>
Chemical structure	
Identification numbers:	
CAS registry	106-99-0
NIOSH RTECS	EI9275000 <sup>c</sup>
EPA hazardous waste	R0377-0754 <sup>d</sup>
DOT/UN/NA/IMDG shipping	1010
EINECS	203-450-8
HSDB	181
NCI	C50602

<sup>a</sup>All information obtained from HSDB 2009 and ChemID Plus Advanced 2009 except where noted.

<sup>b</sup>O'Neil et al. 2006

<sup>c</sup>NIOSH 2005

<sup>d</sup>Miller 1978

CAS = Chemical Abstracts Service; DOT/UN/NA/IMDG = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EINECS = European Inventory of Existing Commercial chemical Substances; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; RTECS = Registry of Toxic Effects of Chemical Substances

## 4. CHEMICAL AND PHYSICAL INFORMATION

**Table 4-2. Physical and Chemical Properties of 1,3-Butadiene**

Property	1,3-Butadiene	Reference
Molecular weight	54.09	O'Neil et al. 2006
Color	Colorless	Lewis 2007
Physical state	Gas	Lewis 2007
Melting point	-108.966 °C	O'Neil et al. 2006
Boiling point	-4.5 °C	O'Neil et al. 2006
Density:		
at 25 °C (g/cm <sup>3</sup> )	0.6149	Lide 2008
Vapor density	1.88 (air=1)	NIOSH 2005
Odor	Mildly aromatic; gasoline-like	Lewis 2007
Water	Not applicable <sup>a</sup>	Amoore and Hautala 1983
Air	1.6 ppm	Amoore and Hautala 1983
Odor threshold		
Solubility:		
Water at 25 °C	735 mg/L	McAuliffe 1966
Organic solvent(s)	Soluble in ether, ethanol and benzene; very soluble in acetone	Lide 2008
Partition coefficients:		
Log K <sub>ow</sub>	1.99	Hansch et al. 1995
K <sub>oc</sub>	288 (estimated) <sup>b</sup>	HSDB 2009
Vapor pressure at 25 °C	2.11x10 <sup>3</sup> mm Hg	AICHe 2000
Henry's law constant at 25 °C	7.4x10 <sup>-2</sup> atm-m <sup>3</sup> /mol (estimated) <sup>c</sup>	HSDB 2009
Autoignition temperature	414 °C	Lewis 2007
Flashpoint	-76 °C	Lewis 2007
Explosive limits	2.0-11.5%	O'Neil et al. 2006
Conversion factors	1 ppm=2.21 mg/m <sup>3</sup> 1 mg/m <sup>3</sup> =0.452 ppm	NIOSH 2005

<sup>a</sup>Amoore and Hautala (1983) reported an odor threshold of 0.0014 ppm for 1,3-butadiene in water; however, these authors state that this solution lacks enough persistence for this value to be used for reference purposes.

<sup>b</sup>This K<sub>oc</sub> value was estimated using the measured log K<sub>ow</sub> value (1.99) and a regression derived equation.

<sup>c</sup>This Henry's Law constant value was calculated from the measured vapor pressure (2.11x10<sup>3</sup> mm Hg at 25 °C) and water solubility (735 mg/L).