4. CHEMICAL AND PHYSICAL INFORMATION

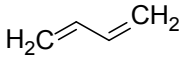
4.1 CHEMICAL IDENTITY

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.

Table 4-1. Chemical Identity of 1,3-Butadiene[a]

Characteristic	Information
Chemical name	1,3-Butadiene
Synonyms and trade names	Butadiene; buta-1,3-diene; biethylene; bivinyl; divinyl; vinylethylene; erythrene; alpha,-gamma-butadiene; pyrrolylene[b]
Chemical formula	C_4H_6
Chemical structure	
Identification numbers:	
CAS registry	106-99-0
NIOSH RTECS	EI9275000[c]
EPA hazardous waste	R0377-0754[d]
DOT/UN/NA/IMDG shipping	1010
EINECS	203-450-8
HSDB	181
NCI	C50602

[a]All information obtained from HSDB 2009 and ChemID Plus Advanced 2009 except where noted.
[b]O'Neil et al. 2006.
[c]NIOSH 2005.
[d]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

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^3)	0.6149	Lide 2008
Vapor density	1.88 (air=1)	NIOSH 2005
Odor	Mildly aromatic; gasoline-like	Lewis 2007
Water	Not applicable[a]	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_{ow}	1.99	Hansch et al. 1995
K_{oc}	288 (estimated)[b]	HSDB 2009
Vapor pressure at 25 °C	$2.11x10^3$ mm Hg	AIChE 2000
Henry's law constant at 25 °C	$7.4x10^{-2}$ atm-m^3/mol (estimated)[c]	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^3 1 mg/m^3=0.452 ppm	NIOSH 2005

[a]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.
[b]This K_{oc} value was estimated using the measured log K_{ow} value (1.99) and a regression derived equation.
[c]This Henry's Law constant value was calculated from the measured vapor pressure ($2.11x10^3$ mm Hg at 25 °C) and water solubility (735 mg/L).