

### 3. CHEMICAL AND PHYSICAL INFORMATION

#### 3.1 CHEMICAL IDENTITY

Data pertaining to the chemical identity of 1,3-butadiene are listed in Table 3-1.

#### 3.2 PHYSICAL AND CHEMICAL PROPERTIES

The physical and chemical properties of 1,3-butadiene are presented in Table 3-2.

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TABLE 3-1. Chemical Identity of 1,3-Butadiene

Characteristic	Information	Reference
Chemical name	1,3-Butadiene	CAS 1989
Synonyms	Butadiene; buta-1,3-diene; biethylene; bivinyl; vinylethylene; erythrene; $\alpha,\alpha$ -butadiene; trans-butadiene; divinyl; pyrrolylene	SANSS 1989; Chemline 1989; HSDB 1989; CAS 1989
Trade name(s)	No data	
Chemical formula	C <sub>4</sub> H <sub>6</sub>	CAS 1989
Chemical structure		
Identification numbers:		
CAS registry	106-99-0	CAS 1989
NIOSH RTECS	EI9275000	SANSS 1989
EPA hazardous waste	R0377-0754	Miller 1978
OHM/TADS	No data	
DOT/UN/NA/IMCO shipping	No data	
HSDB	181	Chemline 1989
NCI	C50602	Chemline 1989

CAS = Chemical Abstracts Service

NIOSH = National Institute for Occupational Safety and Health

RTECS = Registry of Toxic Effects of Chemical Substances

EPA = Environmental Protection Agency

OHM/TADS = Oil and Hazardous Materials Technical Assistance Data Base

DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/  
International Maritime Consultive Organization

HSDB = Hazardous Substance Data Bank

NCI = National Cancer Institute

SANSS = Structure and Nomenclature Search System

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TABLE 3-2. Physical and Chemical Properties of 1,3-Butadiene

Property	Information	Reference
Molecular weight	54.09	Weast et al. 1988
Color	Colorless	Sax and Lewis 1987
Physical state	Gas	Sax and Lewis 1987
Melting point	-108.9°C	Weast et al. 1988
Boiling point		
at 1 atm	-4.4°C	Weast et al. 1988
at 5 atm	47°C	Windholz et al. 1983
at 10 atm	76°C	Windholz et al. 1983
Density (liquid) at 20°C	0.6211 g/mL	Weast et al. 1988
Odor	Mildly aromatic	Sax and Lewis 1987
Odor threshold		
Water	0.0014 mg/L	Amoore and Hautula 1983
Air	1.0-1.6 ppm (recognition) 0.025 ppm (detection)	Amoore and Hautula 1983 Verschueren 1983
Solubility		
Water at 25°C	735 ppm	McAuliffe 1966
Organic solvents	Alcohol, ether, acetone, benzene, polar and nonpolar organic solvents	Weast et al. 1988 Windholz et al. 1983
Partition coefficient		
Log octanol/water	1.99	Hansch and Leo 1985
Log $K_{oc}$ (calculated from $K_{ow}$ )	2.46	Lyman et al. 1982
	2.59	Verschueren 1983
Vapor pressure at 25°C	2100 mmHg	Daubert and Danner 1985
Henry's law constant		
at 25°C (calculated)	$7.05 \times 10^{-2}$ atm-m <sup>3</sup> /mol	Hine and Mookerjee 1975
Autoignition temperature	414°C	Sax and Lewis 1987
Flashpoint	-76°C	Sax and Lewis 1987
Flammability limits		
in air	Extremely flammable	Miller 1978
Conversion factors		
ppm (v/v) to mg/m <sup>3</sup> in air (20°C)	2.21	IARC 1986
mg/m <sup>3</sup> to ppm (v/v) in air (20°C)	0.445	IARC 1986
Bioconcentration factor (calculated from $K_{ow}$ )	19	Lyman et al. 1982
Explosive limits	2-11.5%	Kirshenbaum 1978

