3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Information regarding the chemical identity of 2-butoxyethanol and 2-butoxyethanol acetate is located in Tables 3-l and 3-2, respectively.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

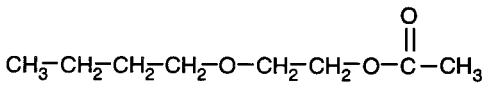
Information regarding the physical and chemical properties of 2-butoxyethanol and 2-butoxyethanol acetate is located in Tables 3-3 and 3-4, respectively.

Table 3-1. Chemical Identity of 2-Butoxyethanol

Characteristic	Information	Reference
Chemical name	2-Butoxyethanol	Merck 1989
Synonyms	Ethylene glycol monobutyl ether; ethylene glycol, butyl ether; ethylene glycol mono-n-butyl ether; ethylene glycol n-butyl ether; monobutyl ethylene glycol ether; monobutyl glycol ether; glycol butyl ether; n-butoxyethanol; 2-butoxy-1-ethanol; butoxyethanol; butyl glycol; butyl oxitol; beta-butoxyethanol; 2-butossi-etanolo (Italian); 2-butoxy-aethanol (German); butoksyetylowy alkohol (Polish); butylglycol (French, German); Butyl Cellosolve; Butyl Cellu-Sol; Caswell No. 121; Chimec NR Ether; Gafcol EB; Dowanol EB; Poly-Solv EB; Ektasolve EB; Eastman EB	Merck 1989 Weast and Astle 1985 HSDB 1995
Registered trade name	Butyl Cellosolve	Merck 1989
Chemical formula	$C_6H_{14}O_2$	Merck 1989
Chemical structure	CH_3-CH_2-CH_2-CH_2-O-CH_2-CH_2-OH	Weast and Astle 1985
Identification numbers:		
CAS Registry	111-76-2	Weast and Astle 1985
NIOSH RTECS	KJ8575000	HSDB 1995
EPA Hazardous Waste	No data	
OHM/TADS	7216719	HSDB 1995
DOT/UN/NA/IMCO	UN 2369 Ethylene glycol monobutyl ether	HSDB 1995
	IMO 6.1 Ethylene glycol monobutyl ether 538	HSDB 1995
HSDB	No data	
NCI	No data	

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances 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

Table 3-2. Chemical Identity of 2-Butoxyethanol Acetate

Characteristic	Information	Reference
Chemical name	2-Butoxyethanol acetate	Sax 1984
Synonyms	Ethylene glycol monobutyl ether acetate; 2-butoxyethanol acetate; acetic acid, 2-butoxyethyl ester; butoxyethyl acetate; butyl glycol acetate; ethylene glycol butyl ether acetate; glycol monobutyl ether acetate; Butyl Cellosolve acetate; Ektasolve EB acetate; Eastman EB Acetate	HSDB 1995
Registered trade name(s)	No data	
Chemical formula	$C_8H_{16}O_3$	Sax 1984
Chemical structure		HSDB 1995
Identification numbers:		
CAS Registry	112-07-2	Sax 1984
NIOSH RTECS	KJ8925000	Sax 1984
EPA Hazardous Waste	No data	
OHM/TADS	No data	
DOT/UN/NA/IMCO	No data	
HSDB	435	HSDB 1995
NCI	No data	

CAS = Chemical Abstracts Services; 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

Table 3-3. Physical and Chemical Properties of 2-Butoxyethanol

Property	Information	Reference
Molecular weight	118.17	Merck 1989
Color	Colorless	Marsden and Mann 1963
Physical state	Liquid	Merck 1989
Melting point	-70 °C -75 °C	HSDB 1995 ASTER 1995a
Boiling point	171 °C at 760 mm Hg 50 °C at 4 mm Hg	Weast 1975 Weast 1989
Density at 20°C	0.9019 g/mL	Merck 1989
Odor	Faint odor Mild ethereal odor	Marsden and Mann 1963 ACGIH 1991
Odor threshold:		
Air	0.10 ppm (v/v) 0.4 ppm (v/v)	Amoore and Hautala 1983 OSHA 1990
Water	No data	
Solubility:		
Water at 25°C	Soluble in all proportions	Riddick and Bunger 1970; Weast 1975
Organic solvent(s)	Miscible with alcohol, ether Soluble in most organic solvents	Weast 1975 Merck 1989
Partition coefficients:		
Log K_{ow}	0.83 0.84	HSDB 1995 ASTER 1995a
Log K_{oc}	1.83 (calculated) 1.79 (calculated)	HSDB 1995; Lyman et al. 1982 ASTER 1995a
Bioconcentration factor		
Log K_{BCF}	0.40 (calculated)	HSDB 1995; Lyman et al. 1982
Vapor pressure		
At 20°C	0.76 mm Hg	HSDB 1995 OSHA 1990
At 25°C	0.88 mm Hg	DOW 1993
Henry's law constant (atm-m^3/mol)	2.08×10^{-8} (calculated) 5.44×10^{-6} (calculated)	Howard 1993; HSDB 1995 ASTER 1995a
Vapor-phase rate constant for reaction with photochemically produced hydroxy radicals	1.96×10^{-11} cm^3/molecule-second at 25°C (estimated)	Atkinson 1987
Atmospheric half-life at 25°C and 5×10^5 hydroxyl radicals/m^3	17 hours (calculated)	HSDB 1995
Autoignition temperature	238°C 244°C	HSDB 1995 Marsden and Mann 1963 ; OSHA 1990

Table 3-3 (*continued*)

Property	Information	Reference
Flashpoint	60°C (closed cup) 62°C (closed cup) 69°C (open cup) 74°C (open cup)	Merck 1989 HSDB 1995 OSHA 1990 Marsden and Mann 1963
Flammability	May be ignited by heat, sparks, or open flame	HSDB 1995
NFPA Classifications	Health = 2[a]; Flammability = 2[b]; Reactivity = 0[c]	HSDB 1995
Conversion factors at 25°C, 1 atm	1 ppm (v/v) = 4.8 mg/m^3 1 mg/m^3 = 0.21 ppm	Calculated Calculated
Explosive limits	1.1% (lower); 10.1% (upper)	OSHA 1990

[a]Materials hazardous to human health. Areas may be entered freely with full-face mask self-contained breathing apparatus which provides eye protection.
[b]Materials must be moderately heated before ignition will occur. Water spray may be used to extinguish the fire because the material can be cooled below its flashpoint.
[c]Materials that (in themselves) are normally stable even under fire exposure conditions and that are not reactive with water. Normal firefighting procedures may be used.

HSDB = Hazardous Substance Data Bank; NFPA = National Fire Protection Association; OSHA = Occupational Safety and Health Administration; Pa = Pascal (133 Pa = 1 mm Hg)

Table 3-4. Physical and Chemical Properties of 2-Butoxyethanol Acetate

Property	Information	Reference
Molecular weight	160.24	Sax 1984
Color	Colorless	Verschueren 1983
Physical state	Liquid	Verschueren 1983
Melting point	-63.5°C	Sax 1984
Boiling point	192.3°C	Verschueren 1983
Density at 20°C	0.94 g/mL	Verschueren 1983
Odor	Fruity	Verschueren 1983
Odor threshold:		
Air	0.1 ppm (absolute threshold) 0.35-0.48 ppm (recognition)	Verschueren 1983 Verschueren 1983
Water	No data	
Solubility:		
Fresh water at 20 °C	11 g/L 1 g/100 g	HSDB 1995 OSHA 1990
Organic solvent(s)	Soluble in hydrocarbons and organic solvents	OSHA 1990
Partition coefficients:		
Log K_{ow}	1.71	ASTER 1995b
Log K_{oc}	1.41 (calculated) 2.27 (calculated)	HSDB 1995 ASTER 1995b
Bioconcentration factor (log K_{BCF})	0.51 (calculated)	HSDB 1995
Vapor pressure at 20°C	0.375 mm Hg 0.579 mm Hg (calculated)	HSDB 1995 ASTER 1995b
Henry's law constant (atm-m^3/mol)	7.19×10^{-6} (calculated) 1.56×10^{-5}	Howard 1993; HSDB 1995 ASTER 1995b
Vapor-phase rate constant with photochemically produced hydroxyl radicals	20.9×10^{-12} cm^3/molecule-second at room temperature (calculated)	Atkinson 1987; HSDB 1995
Atmospheric half-life at 25°C and 5×10^5 hydroxy radicals/m^3	18.4 hours (calculated)	Atkinson 1987; HSDB 1995
Hydrolysis half-life	>1,000 days	ASTER 1995b
Autoignition temperature	340°C	OSHA 1990

Table 3-4 (*continued*)

Property	Information	Reference
Flashpoint	73.9°C (closed cup) 87.8°C (open cup)	OSHA 1990 OSHA 1990
Flammability	Moderate fire hazard when exposed to heat, flame, or oxidizers	HSDB 1995
NFPA Classifications	Health = 1[a] Flammability = 2[b] Reactivity = 0[c]	HSDB 1995 HSDB 1995 HSDB 1995
Conversion factors at 25°C and 1 atm	1 ppm (v/v) = 6.54 mg/m^3 1 mg/m^3 = 0.157 ppm	HSDB 1995 HSDB 1995
Explosive limits	0.88% at 93°C lower; 8.54% at 135°C upper	HSDB 1995

[a]Materials only slightly hazardous to health. It may be desirable to wear self-contained breathing apparatus.
[b]Materials that must be moderately heated before ignition will occur. Water spray may be used to extinguish fire because material can be cooled below its flashpoint.
[c]Materials that (in themselves) are normally stable even under fire exposure conditions and that are not reactive with water. Normal firefighting procedures may be used.

NFPA = National Fire Protection Association