

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Table 3-1 lists common synonyms, trade names and other pertinent identification information for BCEE.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Table 3-2 lists important physical and chemical properties of BCEE.

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TABLE 3-1. Chemical Identity of BCEE

Property	Value	References
Chemical Name	Bis(2-chloroethyl) ether	IARC 1975
Synonyms	1,1'-Oxybis(2-chloro) ethane; bis(chloroethyl) ether; bis(β -chloroethyl)ether; sym-dichloroethylether; 2,2'-dichloro-diethyl ether; 2-dichloroethyl ether; dichloroethyl ether; dichloroethyl oxide; DCEE	IARC 1975
Trade Name	Chlorex	IARC 1975
Chemical Formula	C ₄ H ₈ Cl ₂ O	Weast 1985
Chemical Structure	$ \begin{array}{ccccccc} & \text{H} & \text{H} & & \text{H} & \text{H} & \\ & & & & & & \\ \text{Cl} & - \text{C} & - \text{Cl} & - \text{O} & - \text{C} & - \text{C} & - \text{Cl} \\ & & & & & & \\ & \text{H} & \text{H} & & \text{H} & \text{H} & \end{array} $	
Identification Numbers:		
CAS Registry	111-44-4	NLM 1988
NIOSH RTECS	KN0875000	HSDB 1988
EPA Hazardous Waste	U025	NLM 1988
OHM-TADS	7216672	HSDB 1988
DOT/UN/NA/IMCO Shipping	UN1916	NLM 1988
HSDB	502	NLM 1988
NCI	-- ^a	

CAS - Chemical Abstracts Service
NIOSH - National Institute for Occupational Safety and Health
RTECS - Registry of Toxic Effects of Chemical Substances
OHM-TADS - Oil and Hazardous Materials/Technical Assistance Data System
DOT/UN/NA/IMCO - Department of Transportation/United Nations/North America/
International Maritime Dangerous Goods Code
HSDB - Hazardous Substances Data Bank
NCI - National Cancer Institute

^aNo data located.

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TABLE 3-2. Physical and Chemical Properties of BCEE

Property	Value	References
Molecular Weight	143.04	Weast 1985
Color	colorless, clear	Windholz 1983
Physical State	liquid	Windholz 1983
Melting Point, °C	-24.5	Weast 1985
Boiling Point, °C	178	Weast 1985
Density, 20°/4°	1.2199	Weast 1985
Odor	pungent	Windholz 1983
Odor Threshold		
Air, ppm	0.049	Amoore and Hautala 1983
Solubility		
Water, mg/L	10,700 10,200 17,200	Hake and Rowe 1963 Verschueren 1977 Veith et al. 1980
Organic Solvents	soluble	Weast 1985
Partition coefficients		
Log octanol/water	1.58 1.5 1.1	Callahan et al. 1979 Mabey et al. 1982 Veith et al. 1980
Log k_{oc}	1.1	Mabey et al. 1982
Vapor Pressure, mm Hg, 20 °C	0.71	Verschueren 1977
Henry's law constant, atm-m ³ /mol	1.31E-05	Mabey et al. 1982
Autoignition temperature, °C	369	HSDB 1988
Flash point °C	55	HSDB 1988
Flammability limits	No Data	HSDB 1988
Conversion factors		Verschueren 1977
ppm (v/v) to mg/m ³ in air (25 °C)	1 ppm = 5.85 mg/m ³	
mg/m ³ to ppm (v/v) in air (25 °C)	1 mg/m ³ = 0.17 ppm	

