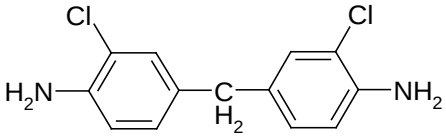
CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of MBOCA is located in Table 4-1.

Table 4-1. Chemical Identity of 4,4'-Methylenebis(2-chloroaniline) (MBOCA)

Characteristic	Information	Reference
Chemical name	4,4'-Methylenebis(2-chloroaniline)	
Synonym(s) and registered trade name(s)[a]	MBOCA, 3,3'-dichloro-4,4'-diaminodiphenylmethane; 4,4'-methylene(bis)-chloroaniline; 4,4'-methylenebis(o-chloroaniline); 4,4'-methylene-bis[2-chlorobenzenamine]; bis(3-chloro-4-aminopropyl) methane; aniline, 4,4'methylene-bis[2-chloro-; bis-(4-amino-3-chlorophenyl) methane; di(4-amino-3-chlorophenyl) methane; bis amine; MCA, CL-MDA; DACPM; Cuamin-M; Activator-M; CA-800; DAC; Bis-Amine A; Curene 442; MOCA; and others	CIS 1992; HSDB 1991; NRC 1981; OHM/TADS 1985; Smith and Woodward 1983
Chemical formula	$C_{13}H_{12}Cl_2N_2$	IARC 1974
Chemical structure		NRC 1981
CAS Registry Number	101-14-4	HSDB 1991

[a]MBOCA trade names that are not in use: Curalin M, Curalon M, Cyanaset, and LD_{813}.

CAS = Chemical Abstracts Service

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of MBOCA is located in Table 4-2.

Table 4-2. Physical and Chemical Properties of 4,4'-Methylenebis(2-chloroaniline) (MBOCA)

Property	Information	Reference
Molecular weight	267	IARC 1974
Color		
Pure form	Colorless crystals	IARC 1974
Technical form	Yellow, tan, or brown pellets	Smith and Woodward 1983; NRC 1981
Physical state	Solid	HSDB 1991
Melting point	110 °C	HSDB 1991
Boiling point	No data	
Density at 20 °C	1.44 g/mL	NRC 1981; Sax and Lewis 1987
Odor	Nearly odorless	NRC 1981
Odor threshold:	No data	
Solubility:		
Water at 24 °C	13.9 mg/L	Voorman and Penner 1986a
Organic solvents	Soluble in hot methyl ethyl ketone, alcohol, acetones, trichloroethylene, toluene, ether, esters, and lipids	HSDB 1991; OHM/TADS 1985; Smith and Woodward 1983
Partition coefficients:		
Log K_{ow}	3.94[a]	HSDB 1991
Log K_{oc}	4810	HSDB 1991
Vapor pressure		
at 25 °C	1.0×10^{-5} mmHg	Smith and Woodward 1983
at 60 °C	1.3×10^{-5} mmHg	NRC 1981
at 100 °C	3.5×10^{-5} mmHg	Smith and Woodward 1983
at 120 °C	5.4×10^{-5} mmHg	NRC 1981
Henry's law constant at 25 °C	4×10^{-11} atm m^3/mole	
Autoignition temperature	No data	
Flashpoint	No data	
Flammability limits	No data	
Conversion factors	No data	
Explosive limits	No data	

[a]Estimated value.