

### **3. CHEMICAL AND PHYSICAL INFORMATION**

#### **3.1 CHEMICAL IDENTITY**

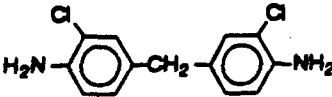
Information regarding the chemical identity of MBOCA is located in Table 3-1.

#### **3.2 PHYSICAL AND CHEMICAL PROPERTIES**

Information regarding the physical and chemical properties of MBOCA is located in Table 3-2.

## 3. CHEMICAL AND PHYSICAL INFORMATION

**TABLE 3-1. Chemical Identity of 4,4'-Methylenebis(2-chloroaniline) (MBOCA)**

| Characteristic                        | Information                                                                                                                                                                                                                                                                                                                                                    | Reference                                                                         |
|---------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------|
| Chemical name                         | 4,4'-Methylenebis(2-chloroaniline)                                                                                                                                                                                                                                                                                                                             |                                                                                   |
| Synonym(s)                            | MBOCA; 3,3'-dichloro-4,4'-diaminodiphenylmethane; 4,4'-methylene(bis)-chloroaniline; 4,4'-methylenebis(o-chloroaniline); 4,4'-methylenebis[2-chlorobenzenamine]; bis(3-chloro-4-aminopropyl) methane; aniline, 4,4'-methylenebis[2-chloro-; bis-(4-amino-3-chlorophenyl) methane; di(4-amino-3-chlorophenyl) methane; bis amine; MCA; CL-MDA; DACPM and others | CIS 1992;<br>HSDB 1991;<br>NRC 1981;<br>OHM/TADS 1985;<br>Smith and Woodward 1983 |
| Registered trade name(s) <sup>a</sup> | Cuamine-M; Activator-M; CA-800; DAC; Bis-Amine A; Curene 442; MOCA                                                                                                                                                                                                                                                                                             | CIS 1992<br>HSDB 1991;<br>OHM/TADS 1985                                           |
| Chemical formula                      | C <sub>13</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub>                                                                                                                                                                                                                                                                                                 | IARC 1974                                                                         |
| Chemical structure                    |                                                                                                                                                                                                                                                                             | NRC 1981                                                                          |
| Identification numbers:               |                                                                                                                                                                                                                                                                                                                                                                |                                                                                   |
| CAS registry                          | 101-14-4                                                                                                                                                                                                                                                                                                                                                       | HSDB 1991                                                                         |
| NIOSH RTECS                           | CY1050000                                                                                                                                                                                                                                                                                                                                                      | HSDB 1991                                                                         |
| EPA hazardous waste                   | U158                                                                                                                                                                                                                                                                                                                                                           | HSDB 1991                                                                         |
| OHM/TADS                              | 8300209                                                                                                                                                                                                                                                                                                                                                        | OHM/TADS 1985                                                                     |
| DOT/UN/NA/IMCO shipping               | No data                                                                                                                                                                                                                                                                                                                                                        |                                                                                   |
| HSDB                                  | 2629                                                                                                                                                                                                                                                                                                                                                           | HSDB 1991                                                                         |
| NCI                                   | No data                                                                                                                                                                                                                                                                                                                                                        |                                                                                   |

<sup>a</sup>MBOCA trade names that are not in use: Curalin M, Curalon M, Cyanaset, and LD 813

CAS = Chemical Abstracts Services; CIS = Chemical Information Systems; 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; NRC = National Research Council (Great Britain); OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

## 3. CHEMICAL AND PHYSICAL INFORMATION

**TABLE 3-2. 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<br>Woodward 1983; NRC<br>1981                     |
| Physical state           | Solid                                                                                                                 | HSDB 1991                                                   |
| Melting point            | 110°C                                                                                                                 | HSDB 1991                                                   |
| Boiling point            | No data                                                                                                               |                                                             |
| Density at 24°C          | 1.44 g/mL                                                                                                             | NRC 1981; Sax and<br>Lewis 1987                             |
| Odor                     | Nearly odorless                                                                                                       | NRC 1981                                                    |
| Odor threshold           | No data                                                                                                               |                                                             |
| Solubility:              |                                                                                                                       |                                                             |
| Water at 24°C            | 13.9 mg/L                                                                                                             | Voorman and Penner<br>1986a                                 |
| Organic solvent(s)       | Soluble in hot methyl ethyl<br>ketone, alcohol, acetones,<br>trichloroethylene, toluene,<br>ether, esters, and lipids | HSDB 1991;<br>OHM/TADS 1985;<br>Smith and<br>Woodward 1983; |
| Partition coefficients:  |                                                                                                                       |                                                             |
| Log $K_{ow}$             | 3.94 <sup>a</sup>                                                                                                     | HSDB 1991                                                   |
| Log $K_{oc}$             | 4,810                                                                                                                 | HSDB 1991                                                   |
| Vapor pressure           |                                                                                                                       |                                                             |
| at 25°C                  | $1.0 \times 10^{-5}$ mmHg                                                                                             | Smith and<br>Woodward 1983                                  |
| at 60°C                  | $1.3 \times 10^{-5}$ mmHg                                                                                             | NRC 1981                                                    |
| at 100°C                 | $3.5 \times 10^{-5}$ mmHg                                                                                             | Smith and<br>Woodward 1983                                  |
| at 120°C                 | $5.4 \times 10^{-5}$ mmHg                                                                                             | NRC 1981                                                    |
| Henry's law constant:    | $4 \times 10^{-11}$ atm m <sup>3</sup> /mole                                                                          | HSDB 1991                                                   |
| Autoignition temperature | No data                                                                                                               |                                                             |
| Flashpoint               | No data                                                                                                               |                                                             |
| Flammability limits      | No data                                                                                                               |                                                             |
| Conversion factors       | No data                                                                                                               |                                                             |
| Explosive limits         | No data                                                                                                               |                                                             |

<sup>a</sup>Estimated value

