# 3. CHEMICAL AND PHYSICAL INFORMATION

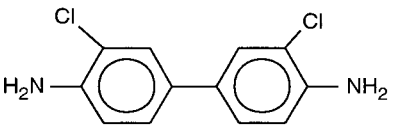
## 3.1 CHEMICAL IDENTITY

Information regarding the chemical identity of 3,3’-dichlorobenzidine is located in Table 3-l.

## 3.2 PHYSICAL AND CHEMICAL PROPERTIES

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

## Table 3-1. Chemical Identity of 3,3'-Dichlorobenzidine

| Characteristic | Information | Reference |
|---|---|---|
| Chemical name | 3,3'-Dichlorobenzidine | Merck 1989 |
| Synonym(s) | Dichlorobenzidine; 3,3'-dichloro(1,1'-biphenyl)-4,4'-diamine; 3,3'-dichloro-4,4'-biphenyldiamine | Merck 1989 |
| Registered trade name(s) | Curithane | IARC 1982a |
| Chemical formula | $C_{12}H_{10}Cl_2N_2$ | Merck 1989 |
| Chemical structure |  | Merck 1989 |
| Identification numbers: | | |
| CAS Registry | 91-94-1 | Merck 1989 |
| NIOSH RTECS | DD0525000 | Chapman & Hall Database 1995 |
| EPA Hazardous Waste | U073 | HSDB 1996 |
| OHM/TADS | 8100004 | HSDB 1996 |
| DOT/UN/NA/IMCO | No data | |
| HSDB | 1632 | HSDB 1996 |
| 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; IARC = International Agency for Research on Cancer

## Table 3-2. Physical and Chemical Properties of 3,3'-Dichlorobenzidine

| Property | Information | Reference |
|---|---|---|
| Molecular weight | 253.13 | Merck 1989 |
| Color | Gray to purple | Merck 1989 |
| Physical state | Crystalline solid | Lewis 1993 |
| Melting point °C | 132–133 | Merck 1989 |
| Boiling point °C | 402 | HSDB 1996 |
| Density at 19 °C | No data | |
| Odor | No data | |
| Odor threshold:<br>Air | No data | |
| Solubility:<br>water at 20 °C<br><br><br>organic solvent(s) | Almost insoluble<br>3.1 mg/L<br>4 mg/L (22 °C)<br>Soluble in alcohol, benzene, Glacial acetic acid | Merck 1989<br>DCMA 1989<br>Banerjee et al. 1978<br>Merck 1989 |
| Partition coefficients: | | |
| Log $K_{ow}$<br><br>Log $K_{oc}$ | 3.21<br>3.5<br>3.2<br>1.43–2.11 at pH7 | SRC 1995b<br>Nyman et al. 1997<br>Mabey et al. 1982<br>HSDB 1996 |
| Vapor pressure at 20 °C | 4.5 x $10^{-9}$ torr | DCMA 1989 |
| Henry's law constant:<br>at 25 °C | 5.11 x $10^{-11}$ atm.$m^3$/mole | SRC 1994 |
| Degradation half-life in air via reaction with OH radicals | 9.7 hours = 39.5704x$10^{-12}$ $cm^3$/molecule-sec | SRC 1995a |
| Dissociation constants<br>$pK_{a,1}$<br>$pK_{a,2}$ | <br>1.6<br>3.2 | <br>Nyman et al. 1997<br>Nyman et al. 1997 |
| Autoignition temperature, °C | No data | |
| Flashpoint | No data | |
| Flammability limits<br>at 25 °C | No data | |
| Conversion factors<br>(25 °C) | ppm = 0.0966 x $mg/m^3$<br>$mg/m^3$ = 10.35 x ppm | IARC 1982a |
| Explosive limits | No data | |