

## **4. CHEMICAL AND PHYSICAL INFORMATION**

### **4.1 CHEMICAL IDENTITY**

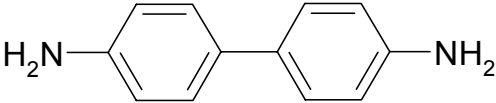
Table 4-1 lists common synonyms, trade names and other pertinent identification information for benzidine.

### **4.2 PHYSICAL AND CHEMICAL PROPERTIES**

Table 4-2 lists important physical and chemical properties of benzidine.

## 4. CHEMICAL AND PHYSICAL INFORMATION

**Table 4-1. Chemical Identity of Benzidine**

| Characteristic           | Information  | Reference                |
|--------------------------|--|--------------------------|
| Chemical name            | Benzidine  | HSDB 1999                |
| Synonym(s)               | 4,4'-Bianiline;<br>4,4'-Diphenyldiamine;<br>4,4'-Diaminobiphenyl;<br>4,4'-Diphenylenediamine;<br>(1,1'-Biphenyl)-4,4'-diamine;<br>C.I. Azoic Diazo Component 112 | IARC 1982a;<br>HSDB 1999 |
| Registered trade name(s) | Fast Corinth Base B  | IARC 1982a               |
| Chemical formula         | C <sub>12</sub> H <sub>12</sub> N <sub>2</sub>   | Lide 1998                |
| Chemical structure       |    |                          |
| Identification numbers:  |  |                          |
| CAS Registry             | 92-87-5  | Lide 1998                |
| NIOSH RTECS              | DC 9625000   | NIOSH 1984c              |
| EPA Hazardous Waste      | U021   | HSDB 1999                |
| OHM/TADS                 | 8100001  | HSDB 1999                |
| DOT/UN/NA/IMCO           | UN 1885  | HSDB 1999                |
| shipping                 | IMO Class 6.1  | HSDB 1999                |
| HSDB                     | 948  | HSDB 1999                |
| NCI                      | C03361   | NLM 1988                 |

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

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**Table 4-2. Physical and Chemical Properties of Benzidine**

| Property                      | Information   | Reference                                    |
|-------------------------------|---|--|
| Molecular weight              | 184.24  | Lide 1998                                    |
| Color                         | Grayish-yellow, white or reddish-gray                             | Lewis 1993                                   |
| Physical state                | Crystalline powder  | Budavari et al. 1996                         |
| Melting point                 | 120 EC  | Lide 1998                                    |
| Boiling point                 | 401 EC  | Lide 1998                                    |
| Specific gravity (20/4 EC)    | 1.250   | Verschuieren 1983                            |
| Odor                          | No data   |  |
| Odor threshold:               |   |  |
| Air                           | No data   |  |
| Water                         | No data   |  |
| pK <sub>a</sub>               | 4.3 (monoprotonated)<br>3.3 (diprotonated)                        | Zierath et al. 1980                          |
| Solubility:                   |   |  |
| Water at 12 EC                | 400 mg/L  | Verschuieren 1983                            |
| at 20 EC                      | 276 mg/L  | EPA 1987b                                    |
| at 25 EC                      | 520 mg/L  | EPA 1987b                                    |
| at 100 EC                     | 9,346 mg/L  | Budavari et al. 1996                         |
| Organic solvent(s)            | 200 g/L (boiling alcohol)<br>20 g/L ether                         | Budavari et al. 1996<br>Budavari et al. 1996 |
| Partition coefficients:       |   |  |
| Log K <sub>ow</sub>           | 1.34  | Hansch et al. 1995                           |
| Log K <sub>oc</sub>           | 1.02–4.9  | EPA 1981b, 1987b; Johnson and Means 1986     |
| Vapor pressure:               |   |  |
| 25 EC                         | 7.0x10 <sup>-7</sup> mmHg   | Neely and Blau 1985                          |
| 20 EC                         | 7.5x10 <sup>-9</sup> mmHg   | Schmidt-Bleik et al. 1982                    |
| Henry's law constant at 25 EC | 5.2x10 <sup>-11</sup> atm·m <sup>3</sup> /mol                     | Meylan and Howard 1991                       |
| Autoignition temperature      | No data   |  |
| Flashpoint                    | No data   |  |
| Flammability limits           | Does not burn or burns with difficulty                            | HSDB 1999                                    |
| Conversion factors at 25 EC   | 1 ppm = 0.133 mg/m <sup>3</sup><br>1 mg/m <sup>3</sup> = 7.52 ppm | IARC 1982a                                   |
| Explosive limits              | No data   |  |

pK<sub>a</sub> = The dissociation constant of the conjugate acid