TITANIUM TETRACHLORIDE 67

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

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

3.2 PHYSICAL AND CHEMICAL PROPERTIES

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

3. CHEMICAL AND PHYSICAL INFORMATION

Table 3-1. Chemical Identity of Titanium Tetrachloride

| Characteristic | Information | Reference |
|--------------------------|--|---------------|
| Chemical name | Titanium tetrachloride | HSDB 1995 |
| Synonym(s) | Tetrachlorotitanium, titanic chloride, titanium chloride, others | HSDB 1995 |
| Registered trade name(s) | No data | |
| Chemical formula | TiCl ₄ | HSDB 1995 |
| Chemical structure | CI CI—Ti— CI CI | OHM/TADS 1992 |
| Identification numbers: | | |
| CAS registry | 7550-45-0 | HSDB 1995 |
| NIOSH RTECS | XR1925000 | HSDB 1995 |
| EPA hazardous waste | No data | HSDB 1995 |
| OHM/TADS | 7217310 | HSDB 1995 |
| DOT/UN/NA/IMCO shipping | IMCO/UN: #8.0/1838; DOT: #1838 | CHRIS 1985 |
| HSDB | 870 | HSDB 1995 |
| NCI | No data | |

CAS = Chemical Abstracts Service; CHRIS = Chemical Hazards Response Information System; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substance 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

3. CHEMICAL AND PHYSICAL INFORMATION

Table 3-2. Physical and Chemical Properties of Titanium Tetrachloride

| Property | Information | Reference |
|-----------------------------------|--|-----------------------------|
| Molecular weight | 189.70 | Sax and Lewis 1989 |
| Color | Colorless | Merck 1989 |
| Physical state | Liquid | CHRIS 1985 |
| Melting point | –24.1 °C | Merck 1989 |
| | –24 °C | NFPA 1994 |
| Boiling point | 136.4 °C | Merck 1989 |
| Density: | | |
| at 20 °C | 1.726 g/cm ³ | Merck 1989 |
| Odor | Penetrating acid odor | Merck 1989 |
| Odor threshold: | | |
| Water | No data | |
| Air | No data | |
| Solubility: | | |
| Water at 20 °C | Soluble in cold water | Merck 1989 |
| | Reacts | NFPA 1994 |
| Organic solvent(s) | Soluble in alcohol | Merck 1989 |
| Partition coefficients: | NI- daka | |
| Log K _{ow} | No data No data | |
| Log K _{oc} | NO data | |
| Vapor pressure at 20 °C | 10.0 mm Ua | Whitehood 1092 |
| at 20 °C at 22 °C | 10.0 mm Hg 9.6 mm Hg | Whitehead 1983 NFPA 1994 |
| | 5.6 mm rig | 1411 A 1004 |
| Henry's law constant: at 20 °C | No data | |
| at 30 °C | No data | |
| Autoignition temperature | No data | |
| Flashpoint | No data | |
| Flammability limits | Nonflammable | OHM/TADS 1992 |
| Conversion factors | 1 mg/m ³ = 7.76 ppm ^a 1 ppm = 0.129 mg/m ³ | Calculated Calculated |
| Explosive limits | Reactive only under extreme conditions | OHM/TADS 1992 |

 $^{^{}a}$ 1 mg/m 3 = 1 ppm × 189.70/24.45

CHRIS = Chemical Hazards Response Information System; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; NFPA = National Fire Protection Association