# 3. CHEMICAL AND PHYSICAL INFORMATION

## 3.1 CHEMICAL IDENTITY

*n*-Hexane is a very volatile aliphatic hydrocarbon. It is a constituent in the paraffin fraction of crude oil and natural gas and is also used as an industrial chemical and laboratory reagent. Laboratory grade *n*-hexane contains approximately 99% *n*-hexane. *"*Hexane*"* or *"*hexanes*"* is a commercial and industrial product consisting of a mixture of hydrocarbons with six carbon atoms and includes *n*-hexane and its isomers 2-methylpentane and 3-methylpentane as well as small amounts of other hydrocarbons (Brugnone et al.1991). Laboratory and industrial solvents such as *"*hexane*"* and petroleum ether contain *n*-hexane from <0.1% to as much as 33% (Creaser et al.1983). Information regarding the chemical identity of *n*-hexane is located in Table 3-1.

Many commercial grades of *n*-hexane contain appreciable amounts of other hydrocarbons in addition to *n*-hexane (for instance, toluene or such solvents as acetone or methyl ethyl ketone; see below for other chemicals in such mixtures). Various types of commercial grades of *n*-hexane are available, and the constituents besides *n*-hexane are usually an intentional part of the process for preparing these commercial mixtures. Where intended for specialized oil extraction or laboratory uses, the purity of the *n*-hexane products may be in the range of 95-99% *n*-hexane; for a variety of uses where purity is not as important, commercial *n*-hexane mixtures (in the range of 20-80% of *n*-hexane) may contain small amounts of chemicals such as acetone, methyl ethyl ketone, dichloromethane, and trichloroethylene, aromatics such as toluene, and other types of petroleum hydrocarbons (Jorgensen and Chor 1981; Takeuchi et al.1993). In commercial grades of *n*-hexane, some of the constituents are purposefully added as denaturants, often to discourage the abuse of the chemical to induce *"*highs*"* through sniffing or inhalation (Altenkirch et al. 1982).

## 3.2 PHYSICAL AND CHEMICAL PROPERTIES

The National Fire Protection Association (NFPA) has assigned *n*-hexane a health hazard identification code of 1 (slight) and flammability code of 3 (serious) (NFPA 1994). *n*-Hexane is flammable and may be ignited by heat, sparks, and flames. Flammable vapor may spread away from a spill. The vapor may be an explosion hazard. *n*-Hexane can react vigorously with oxidizing materials such as liquid chlorine, concentrated oxygen, and sodium hypochlorite. *n*-Hexane will attack some forms of plastics, rubber, and coatings. Information regarding the physical and chemical properties of hexane is located in Table 3-2.

## Table 3-1. Chemical Identity of *n*-Hexane

| Characteristic | Information | Reference |
|---|---|---|
| Chemical name | *n*-Hexane | Merck 1989 |
| Synonym(s) | Hexane<br>Hexyl hydride | HSDB 1996<br>NFPA 1994 |
| Registered trade name(s) | Skellysolve B<br>Gettysolve-B | HSDB 1996<br>RTECS 1997 |
| Chemical formula | $C_6H_{14}$ | Lide 1994 |
| Chemical structure | $CH_3CH_2CH_2CH_2CH_2CH_3$ | |
| Identification numbers: | | |
| CAS Registry | 110-54-3 | ASTER 1995 |
| NIOSH RTECS | MN9275000 | RTECS 1997 |
| EPA Hazardous Waste | No data | |
| OHM/TADS | No data | |
| DOT/UN/NA/IMCO | UN 1208; IMO 3.1 | HSDB 1996 |
| HSDB | 91 | HSDB 1996 |
| NCI | C60571 | HSDB 1996 |

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 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

## Table 3-2. Physical and Chemical Properties of *n*-Hexane

| Property | Information | Reference |
|---|---|---|
| Molecular weight | 86.18 | Lide 1994 |
| Color | Colorless | Merck 1989 |
| Physical state | Liquid | Merck 1989 |
| Melting point | -95 °C | Lide 1994 |
| Boiling point | 69 °C | Lide 1994 |
| Density | 0.6603 at 20 °C | Lide 1994 |
| Odor | Faint, peculiar odor | Merck 1989 |
| Odor threshold: | | |
| Water | 0.0064 mg/L | Amoore and Hautala 1983 |
| Air | 130 ppm | Amoore and Hautala 1983 |
| Solubility: | | |
| Water | Insoluble | Merck 1989 |
| | 9.5 mg/L | Chiou et al. 1988 |
| Organic solvent(s) | Miscible with alcohol, chloroform, ether | Merck 1989 |
| Partition coefficients: | | |
| Log $K_{ow}$ | 3.290 | SRC 1995 |
| Log $K_{oc}$ | 2.90 | Coates et al. 1985 |
| | 3.10–3.61(est.) | HSDB 1996 |
| Vapor pressure | 150 mm Hg at 25 °C | HSDB 1996 |
| | 138 mm Hg at 24 °C | Chiou et al. 1988 |
| Henry's law constant: at 25 °C | 1.69 atm-$m^3$/mole | SRC 1994a |
| Autoignition temperature | 225 °C | NFPA 1994 |
| Flashpoint | -22 °C | NFPA 1994 |
| Flammability limits at 25 °C | 1.1–7.5 % | NFPA 1994 |
| Conversion factors | | |
| ppm to $mg/m^3$ | 1 $mg/m^3$ = 0.284 ppm | HSDB 1996 |
| $mg/m^3$ to ppm | 1 ppm = 3.52 $mg/m^3$ | |
| Explosive limits | 1.1–7.5% | WHO 1991 |