

CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 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 solvent. 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 presented in Table 4-1.

Table 4-1. Chemical Identity of *n*-Hexane

Characteristic	Information	Reference
Chemical name	<i>n</i> -Hexane	Budavari et al. 1989
Synonym(s) and registered trade name(s)	Hexane Hexyl hydride Skellysolve B Gettysolve-B	IUPAC name NFPA 1991 NLM 2023 NLM 2023
Chemical formula	C ₆ H ₁₄	Lide 2005
SMILES	CCCCCC	NLM 2023
Chemical structure	CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ CH ₃	
CAS Registry Number	110-54-3	NLM 2023

CAS = Chemical Abstracts Service; SMILES = simplified molecular-input line-entry system

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 MEK; 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, MEK, dichloromethane, 2- or 3-methylpentane, 2,3-dimethylbutane, cyclohexane, methyl cyclopentane, trichloroethylene, aromatics such as toluene, and other types of petroleum hydrocarbons (Jørgensen and Cohr 1981; Takeuchi et al. 1993; WHO 1991). In commercial grades of *n*-hexane, some

4. CHEMICAL AND PHYSICAL INFORMATION

of the constituents are purposefully added as denaturants, often to discourage the misuse of the chemical to induce “highs” through sniffing or inhalation (Altenkirch et al. 1982).

4.2 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 1991). *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. Virtually all *n*-hexane is obtained from petroleum mixtures through controlled fractional distillation and other refinery-based processes (Speight 2006). The presence of many types of hydrocarbon impurities in many commercial grades of *n*-hexane, combined with the intentional denaturing of *n*-hexane preparations to discourage substance misuse, make it difficult to establish odor thresholds for many products containing *n*-hexane. Information regarding the physical and chemical properties of *n*-hexane is presented in Table 4-2.

Table 4-2. Physical and Chemical Properties of *n*-Hexane

Property	Information	Reference
Molecular weight	86.18	Lide 2005
Color	Colorless	Budavari et al. 1989
Physical state	Liquid	Budavari et al. 1989
Melting point	-95°C	Lide 2005
Boiling point	69°C	Lide 2005
Density at 20°C	0.6606 g/cm ³	Lide 2005
Odor	Faint, peculiar odor	Budavari et al. 1989
Odor threshold:		
Water	0.0064 mg/L	Amoore and Hautala 1983
Air	130 ppm	Amoore and Hautala 1983
Taste threshold	No data	
Solubility:		
Water	Insoluble 9.5 mg/L	Budavari et al. 1989 NLM 2023
Organic solvent(s)	Miscible with alcohol, chloroform, ether	Budavari et al. 1989
Partition coefficients:		
Log K _{ow}	3.90, 2.90	Coates et al. 1985; Hansch et al. 1995

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-2. Physical and Chemical Properties of *n*-Hexane

Vapor pressure	138 mmHg at 24°C	Chiou et al. 1988
Henry's law constant at 25°C	1.003 atm-m ³ /mole 1.3 atm-m ³ /mole	Ashworth et al. 1988 Zhu et al. 2004
Autoignition temperature	225°C	NFPA 1991
Flashpoint	-22°C	NFPA 1991
Flammability limits	1.1–7.5%	NFPA 1991
Explosive limits	1.1–7.5%	WHO 1991
Conversion factors	1 ppm = 3.52 mg/m ³ 1 mg/m ³ = 0.284 ppm	WHO 1991