3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

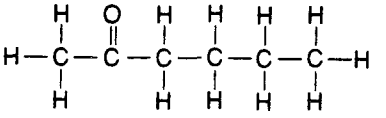
Table 3-1 lists common synonyms, trade names, and other pertinent identification information for 2-hexanone.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Table 3-2 lists important physical and chemical properties of 2-hexanone.

3. CHEMICAL AND PHYSICAL INFORMATION

TABLE 3-1. Chemical Identity of 2-Hexanone

Characteristic	Information	Reference
Chemical name	2-Hexanone	Sax 1984
Synonyms	Methyl n-butyl ketone; 2-oxohexane; n-butyl methyl ketone; propylacetone	NLM 1989; Sax and Lewis 1987
Trade names	No data	
Chemical formula	$C_6H_{12}O$	Windholz 1983
Chemical structure		ACGIH 1986
Identification numbers:		
CAS registry	591-78-6	Sax and Lewis 1987
NIOSH RTECS	MP1400000	Sax 1984
EPA hazardous waste	No data	
OHM/TADS	No data	
DOT/UN/NA/IMCO shipping	No data	
HSDB	543	HSDB 1989
NCI	No data	

CAS = Chemical Abstracts Service; 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

TABLE 3-2. Physical and Chemical Properties of 2-Hexanone

Property	Information	Reference
Molecular weight	100.16	Windholz 1983
Color	Colorless	Windholz 1983
Physical state	Liquid	Windholz 1983
Melting point	-57°C	Weast 1985
Boiling point	128°C	Weast 1985
Density at 20°C	0.83	Windholz 1983
Odor	Similar to acetone	EPA 1981
Odor threshold:		
Water	0.25 mg/L	Amoore and Hautala 1983
Air	0.076 ppm (0.31 mg/m^3)	Amoore and Hautala 1983
Solubility:		
Water at 20°C	20,000-35,000 mg/L	Morrison and Boyd 1974; Verschueren 1983
Organic solvents	Soluble in alcohol, ether, acetone	Weast 1985
Partition coefficients:		
Log octanol/water	1.38	EPA 1981
Log K_{oc}	No data	
Vapor pressure at 25°C	11.6 mmHg	Ambrose et al. 1975
Henry's law constant: at 20°C	No data	
Autoignition temperature	991°F (533°C)	Sax 1984
Flashpoint	95°F (35°C)(open cup)	Sax 1984
	163°F(73°C)(closed cup)	EPA 1981
Flammability limits	No data	
Conversion factors	1 ppm = 4.097 mg/m^3 (calculated)	
	1 mg/m^3 = 0.244 ppm (calculated)	
Explosive limits	1.2%-8%	Sax and Lewis 1987