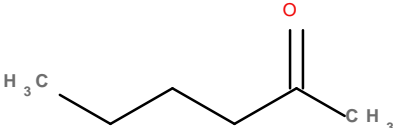


CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Table 4-1 lists common synonyms, trade names, and other pertinent identification information for 2-hexanone. Note that the purity of commercial-grade 2-hexanone ranges from 70 to 96%; contaminants may include methyl isobutyl ketone (MiBK) (Topping et al. 2001).

Table 4-1. Chemical Identity of 2-Hexanone^a

Characteristic	Information
Chemical name	2-Hexanone
Synonym(s) and registered trade name(s)	Methyl <i>n</i> -butyl ketone; MBK; 2-oxohexane; <i>n</i> -butyl methyl ketone, propylacetone; MnBK
Chemical formula	C ₆ H ₁₂ O
Chemical structure	
CAS Registry Number	591-78-6

^aAll information obtained from HSDB (2009), unless otherwise noted.

CAS = Chemical Abstracts Service

4.2 PHYSICAL AND CHEMICAL PROPERTIES

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

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-2. Physical and Chemical Properties of 2-Hexanone

Property	Information
Molecular weight	100.16
Color	Colorless
Physical state	Liquid
Melting point	-55.5°C
Boiling point	127.2°C
Density at 20°C	0.83
Odor	Similar to acetone, but more pungent
Odor threshold:	
Water	0.25 mg/L
Air	0.076 ppm (0.31 mg/m ³)
Solubility:	
Water at 20°C	1.72x10 ⁴ mg/L
Organic solvents	Soluble in acetone; miscible in ethanol and ether
Partition coefficients:	
Log K _{ow}	1.38
Log K _{oc}	No data
Vapor pressure at 25°C	11.6 mm Hg
Henry's law constant	9.32x10 ⁻⁵ atm-m ³ /mol at 25°C (estimated)
Autoignition temperature	795°F (423°C)
Flashpoint	95°F (35°C) (open cup); 77°F (25°C) (closed cup)
Flammability limits	1.2–8%
Conversion factors at 25°C, 760 mm Hg	1 ppm=4.10 mg/m ³ 1 mg/L=244 ppm
Explosive limits	1.22–8%

Source: HSDB 2009