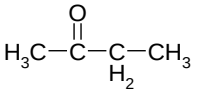
CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Data pertaining to the chemical identity of 2-butanone are listed in Table 4-1.

Table 4-1. Chemical Identity of 2-Butanone

Characteristic	Information	Reference
Chemical name	2-Butanone	CAS 1989
Synonym(s) and registered trade name(s)	Methyl ethyl ketone; MEK; ethyl methyl ketone; methyl acetone; and others; Meetco	CAS 1989; SANSS 1989; Chemline 1989; OHM/TADS 1989
Chemical formula	C_4H_8O	CAS 1989
Chemical structure		
CAS Registry Number	78-93-3	CAS 1989

CAS = Chemical Abstracts Service

4.2 PHYSICAL AND CHEMICAL PROPERTIES

The physical and chemical properties of 2-butanone are presented in Table 4-2.

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

Property	Information	Reference
Molecular weight	72.11	Weast et al. 1988
Color	Colorless	Sax and Lewis 1987
Physical state	Liquid	Sax and Lewis 1987
Melting point	-86.3°C	Weast et al. 1988
Boiling point	79.6°C	Weast et al. 1988
Density (liquid) at 20°C	0.8054	Weast et al. 1988
Odor	Acetone-like	Sax and Lewis 1987
Odor threshold:		
Water	8.4 ppm	Amoore and Hautala 1983
Air	5.4 ppm	Amoore and Hautala 1983
Solubility:		
Water at 25°C	136,000 mg/L	Tewari et al. 1982
Organic solvents	Benzene, alcohol, ether, oils, most organic solvents	Sax and Lewis 1987; Neier and Strehlke 1985

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

Property	Information	Reference
Partition coefficients:		
Log K_{ow}	0.29	Hansch and Leo 1985
Log K_{oc}	0.55	Roy and Griffin 1985
Vapor pressure at 25°C	90.6 mmHg	Riddick et al. 1986
Henry's law constant at 25°C	5.77×10^{-5} atm m^3/mol	Rathburn and Tai 1987
Autoignition temperature	515°C	Sax and Lewis 1987
Flashpoint:		
Closed cup	-2°C	Riddick et al. 1986
Open cup	1°C	Riddick et al. 1986
Flammability limits in air	2–10%	Sax and Lewis 1987
Conversion factors:		
ppm (v/v) to mg/m^3 in air (20°C)	1 ppm=2.93 mg/m^3	
mg/m^3 to ppm (v/v) in air (20°C)	1 mg/m^3=0.341 ppm	
Bioconcentration factor	0.98 (calculated from K_{ow})	Lyman et al. 1982
Explosive limits	No data	