

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Data pertaining to the chemical identity of 2-butanone are listed in Table 3-1.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

The physical and chemical properties of 2-butanone are presented in Table 3-2.

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TABLE 3-1. Chemical Identity of 2-Butanone

Characteristic	Information	Reference
Chemical name	2-Butanone	CAS 1989
Synonyms	Methyl ethyl ketone; MEK; ethyl methyl ketone; methyl acetone; and others	CAS 1989; SANSS 1989; Chemline 1989
Trade name(s)	Meetco	OHM/TADS 1989
Chemical formula	C ₄ H ₈ O	CAS 1989
Chemical structure	$\begin{array}{c} \text{O} \\ \\ \text{CH}_3 - \text{C} - \text{CH}_2 - \text{CH}_3 \end{array}$	
Identification numbers:		
CAS registry	78-93-3	CAS 1989
NIOSH RTECS	EL6475000	HSDB 1989
EPA hazardous waste	U159	HSDB 1989
OHM/TADS	7216796	Chemline 1989
DOT/UN/NA/IMCO	UN1193, UN1232	Chemline 1989
HSDB	99	HSDB 1989
NCI	No data	

CAS = Chemical Abstracts Service

EPA = Environmental Protection Agency

DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/
International Maritime Consultive Organization

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 Base

RTECS = Registry of Toxic Effects of Chemical Substances

SANSS = Structure and Nomenclature Search System

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TABLE 3-2. 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
Partition coefficient		
Log octanol/water	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 Louis 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	

