

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Data pertaining to the chemical identities of acetone, the simplest aliphatic ketone, are listed in Table 3-1.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

The physical and chemical properties of acetone are given in Table 3-2. The physical properties of acetone, such as high evaporation rate, low viscosity, and miscibility with water and several organic solvents make it suitable for use as a solvent (Krasavage et al. 1982). Because of its ability to undergo addition, oxidation/reduction, and condensation reactions, acetone is used as a raw material in the chemical synthesis of many commercial products (Nelson and Webb 1978).

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TABLE 3-1. Chemical Identity of Acetone

Characteristic	Information	Reference
Chemical name	Acetone	HSDB 1992
Synonym(s)	Dimethyl ketone; 2-propanone; beta-ketopropane	HSDB 1992
Registered trade name(s)	No data	
Chemical formula	C ₃ H ₆ O	
Chemical structure	$\begin{array}{c} \text{O} \\ \\ \text{CH}_3\text{-C-CH}_3 \end{array}$	
Identification numbers:		
CAS registry	67-64-1	HSDB 1992
NIOSH RTECS	AL3150000	HSDB 1992
EPA hazardous waste	U002; F003	HSDB 1992
OHM/TADS	7216568	HSDB 1992
DOT/UN/NA/IMCO shipping	UN1090	HSDB 1992
HSDB	41	HSDB 1992
NCI	ND	HSDB 1992

CAS = Chemical Abstracts Services; 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

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TABLE 3-2. Physical and Chemical Properties of Acetone

Property	Information	Reference
Molecular weight	58.08	Riddick et al. 1986
Color	Colorless	HSDB 1992
Physical state	Liquid	HSDB 1992
Melting point	-95.35°C	HSDB 1992
Boiling point	56.2°C at 1 atm	HSDB 1992
Density:		
at 20°C	0.78998 g/mL	Riddick et al. 1986
at 25°C	0.78440 g/mL	Riddick et al. 1986
at 30°C	0.78033 g/mL	Riddick et al. 1986
Odor	Mildly pungent and aromatic	Nelson and Webb 1978
Odor threshold:		
Water	20 ppm (w/v)	Amoore and Hautala 1983
Air (absolute)	13-20 ppm (v/v)	Amoore and Hautala 1983; Hellman and Small 1974
100% odor recognition	100-140 ppm	Hellman and Small 1974; Leonardos et al. 1969
Solubility:		
Water at 20°C	Completely miscible	HSDB 1992
Organic solvent(s)	Soluble in benzene and ethanol	HSDB 1992
Partition coefficients:		
Log K_{ow}	-0.24 (recommended value)	Collander 1951; Sangster 1989
Log K_{oc}	0.73 (estimated) ^a	Lyman 1982
Vapor pressure at 20°C	181.72 mmHg	Riddick et al. 1986
Henry's law constant:		
at 25°C	4.26×10^{-5} atm·m ³ /mol	Rathbun and Tai 1987
Autoignition temperature	465°C	HSDB 1992
Flashpoint (closed cup)	-20°C	HSDB 1992
Flammability limits		HSDB 1992
in air at 25°C	Lower, 2.15%; upper, 13.0%	
Conversion factors:		
in air at 25°C	1 ppm = 2.374 mg/m ³	HSDB 1992
Explosive limits		HSDB 1992
Lower, 2.6% in air (v/v);		
upper, 12.8% in air (v/v)		HSDB 1992

^aEstimated by regression equation 4-13 in Lyman (1982)

w/v = weight per volume; v/v = volume per volume

