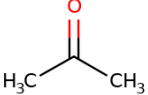


CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Table 4-1 lists common synonyms, trade names, and other pertinent identification information for acetone.

Table 4-1. Chemical Identity of Acetone

Characteristic	Information	Reference
Chemical name	Acetone	PubChem 2021
Synonym(s) and registered trade name(s)	Dimethyl ketone; 2-propanone; propan-2-one; beta-ketopropane	PubChem 2021
Chemical formula	C ₃ H ₆ O	Haynes et al. 2015
Chemical structure		Haynes et al. 2015
CAS Registry Number	67-64-1	Haynes et al. 2015

CAS = Chemical Abstracts Service

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Acetone is a colorless volatile liquid with a fruity odor and pungent, sweetish taste. It dissolves completely in water and is expected to volatilize from soil and water. Table 4-2 lists important physical and chemical properties of acetone.

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-2. Physical and Chemical Properties of Acetone

Property	Information	Reference
Molecular weight	58.079	Haynes et al. 2015
Color	Colorless	PubChem 2021
Physical state	Liquid	Haynes et al. 2015
Melting point	-94.9°C	Haynes et al. 2015
Boiling point	56.08°C	Haynes et al. 2015
Critical temperature and pressure	508.1 K and 4.7 MPa	Haynes et al. 2015
Density at 20°C	0.7845 g/cm ³ at 25°C	Haynes et al. 2015
Taste	Pungent, sweetish	PubChem 2021
Odor	Fruity odor	PubChem 2021
Odor threshold:		PubChem 2021
Water	20 ppm, w/v	
Air	13 ppm, v/v	
Solubility:		
Water at 20°C	Miscible with water	Haynes et al. 2015
Organic solvents	Miscible with ethanol, diethyl ether, acetone, benzene, chloroform	
Partition coefficients:		
Log K _{ow}	-0.24	Haynes et al. 2015
Log K _{oc}	0.73 (estimated) ^a	Lyman 1982
Vapor pressure at 20°C		Haynes et al. 2015
Henry's law constant at 25°C		PubChem 2021
Degradation half-life in air via reaction with OH radicals	1.80x10 ⁻¹³ cm ³ /molecule-second at 25°C	PubChem 2021
Dissociation constant	pKa 20	PubChem 2021
Heat of vaporization	30.99 kJ/mol at 25°C	Haynes et al. 2015
Autoignition temperature	465°C	Haynes et al. 2015
Flashpoint	-20°C	Haynes et al. 2015
Flammability limits in air (percent by volume)	2.5–12.8%	Haynes et al. 2015
Conversion factors	1 ppm = 2.38 mg/m ³ 1 mg/m ³ = 0.42 ppm	
Incompatibilities and reactivity	Acetone and chloroform is a potentially explosive combination in the presences of a base; incompatible with nitric and sulfuric acid mixtures and hydrogen peroxide	Haynes et al. 2015

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