## **CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION**

## 4.1 CHEMICAL IDENTITY

Data pertaining to the chemical identity of vinyl acetate are listed in Table 4-1.

Characteristic	Information	Reference
Chemical name	Vinyl acetate	Windholz 1983
Synonym(s) and registered trade name(s)	Acetic acid, ethenyl ester; acetic acid ethylene ester; acetic acid, vinyl ester; 1-acetoxyethylene; ethanoic acid; ethenyl ester; ethenyl acetate; ethenyl ethanoate; vinyl A monomer; vinyl ethanoate; VAC; vinyl acetate HQ; VYAC; ZESET T	NLM 2022
Chemical formula	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	Windholz 1983
SMILES	CC(=O)OC=C	NLM 2022
Chemical structure	$\begin{array}{cccc} H & O & H & H \\ H & H & H \\ H - C - C - O - C = C \\ H & H \end{array}$	IARC 1979
CAS Registry Number	108-05-4	NLM 2022
InChIKey	XTXRWKRVRITETP-UHFFFAOYSA-N	NLM 2022
InChl	1S/C4H6O2/c1-3-6-4(2)5/h3H,1H2,2H3	NLM 2022

## Table 4-1. Chemical Identity of Vinyl Acetate

CAS = Chemical Abstracts Service; SMILES = simplified molecular-input line-entry system

## 4.2 PHYSICAL AND CHEMICAL PROPERTIES

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

Property	Information	Reference
Molecular weight	86.09 g/mol	Windholz 1983
Color	Colorless	U.S. Coast Guard 1978
Physical state	Liquid (polymerizes into a transparent, colorless solid in light)	Windholz 1983 NLM 2022
Melting point	-93.2°C	NLM 2022
Boiling point	72–73°C	NLM 2022
Density at 20 °C	0.932 (20/4°C)	NLM 2022
Relative vapor density (air=1)	3.0	NLM 2022
Odor	Sweet smell in small quantities, pleasant fruity characteristic	U.S. Coast Guard 1978
Odor threshold:		
Water	0.88 ppm (w/v) 0.25 ppm	Amoore and Hautala 1983 Goeva 1966
Air	0.5 ppm (v/v) 0.12 ppm	Amoore and Hautala 1983 U.S. Coast Guard 1978
Solubility:		
Water at 20 °C	2.0x10⁴ mg/L 1 g/100 mL	EPA 2012 Windholz 1983
Organic solvents	10% solubility in alcohol, ether, and benzene	NLM 2022
Partition coefficients:		
Log K <sub>ow</sub>	0.21–0.73	Fujisawa and Masuhara 1981; Howard 1989
Log Koc	0.75 (estimated, MCI Method) 1.3 (estimated, K <sub>ow</sub> Method)	EPA 2012
Vapor pressure at 20 °C	83 mmHg (115 mmHg at 25°C; 140 mmHg at 30°C)	Verschueren 1983
Henry's law constant at 25 °C	5.11x10 <sup>-4</sup> atm-m <sup>3</sup> /mol <sup>-1</sup> (calculated) <sup>a</sup>	NLM 2022
Autoignition temperature	402°C 426.6°C	NFPA 1994 Hawley 1981
Flashpoint	-8°C (closed cup); -1.1°C (Tag open cup)	Hawley 1981; Windholz 1983
Flammability limits	2.6–13.4% by volume	NFPA 1994
Conversion factors	1 ppm=3.52 mg/m <sup>3</sup> 1 mg/m <sup>3</sup> =0.28 ppm	
Explosive limits <sup>b</sup>	2.6–13.4%	NLM 2022

<sup>a</sup>Henry's law constant = vapor pressure/water solubility. <sup>b</sup>Explosive in water and air.

w/v = percent "weight in volume;" v/v = percent "volume in volume"