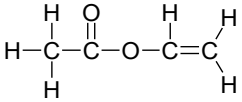
CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of vinyl acetate, also commonly referred to as ethenyl acetate (International Union of Pure and Applied Chemistry [IUPAC] name) or ethenyl ethanoate is presented in Table 4-1. It is the acetate ester of vinyl alcohol.

Table 4-1. Chemical Identity of Vinyl Acetate

Characteristic	Information	Reference
Chemical name	Vinyl acetate	NLM 2022
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	$C_4H_6O_2$	NLM 2022
SMILES	CC(=O)OC=C	NLM 2022
Chemical structure		NLM 2022
CAS Registry Number	108-05-4	NLM 2022
InChIKey	XTXRWKRVRITETP-UHFFFAOYSA-N	NLM 2022
InChI	1S/C4H6O2/c1-3-6-4(2)5/h3H,1H2,2H3	NLM 2022

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

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Vinyl acetate is a flammable, volatile colorless liquid. Pure vinyl acetate that is not produced with inhibitors may polymerize on exposure to light. Information regarding physical and chemical properties of vinyl acetate is presented in Table 4-2.

Table 4-2. Physical and Chemical Properties of Vinyl Acetate

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	2.0×10^4 mg/L 1 g/50 mL	EPA 2012 Windholz 1983
Organic solvents	10% solubility in alcohol, ether, and benzene	NLM 2022
Partition coefficients:		
Log K_{ow}	0.21–0.73	Fujisawa and Masuhara 1981; Howard 1989
Log K_{oc}	0.75 (estimated, MCI Method) 1.3 (estimated, K_{ow} Method)	EPA 2012
Vapor pressure at 20 °C	83 mmHg at 20°C 115 mmHg at 25°C 140 mmHg at 30°C	Verschueren 1983
Henry's law constant at 25 °C	5.11×10^{-4} atm-m^3/mol^{-1} (calculated)[a]	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^3 1 mg/m^3=0.28 ppm	
Explosive limits[b]	2.6–13.4%	NLM 2022

[a]Henry's law constant = vapor pressure/water solubility.
[b]Explosive in water and air.

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