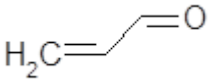
CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Acrolein is the smallest unsaturated aldehyde with a molecular formula of C_3H_4O; its chemical structure consists of one aldehyde group (C=O) and one carbon-carbon double bond (C=C). Information regarding the chemical identity of acrolein is presented in Table 4-1.

Table 4-1. Chemical Identity of Acrolein

Characteristic	Information	Reference
Chemical name	Acrolein	
Synonym(s) and registered trade name(s)	Acraldehyde, acrylic aldehyde, acrylaldehyde, allyl aldehyde, ethylene aldehyde, 2-propenal, propenaldehyde, Aqualin, Biocide, Crolean, MAGNACIDE B®, MAGNACIDE H®, Slimicide	NLM 2024; RTECS 2019
Chemical formula	C_3H_4O	NLM 2024
SMILES	C=CC=O	NLM 2024
Chemical structure		
CAS Registry Number	107-02-8	NLM 2024

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

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Acrolein is a liquid and may be colorless or yellowish depending on its purity. It is a volatile organic compound (VOC) with a pungent, choking odor. Acrolein is soluble in water and miscible with certain organic solvents. Information regarding physical and chemical properties of acrolein is presented in Table 4-2.

Table 4-2. Physical and Chemical Properties of Acrolein

Property	Information	Reference
Molecular weight	56.06	O'Neil 2013
Color	Colorless or yellowish	Lewis 1997
Physical state	Liquid	Lewis 1997
Melting point	-87.8 °C	NLM 2024
Boiling point	52.3 °C	NLM 2024
Density at 20°C	0.840 g/cm^3	NLM 2024
Odor	Disagreeable, choking odor, pungent	Lewis 1997; O'Neil 2013
Odor threshold:		
Water	0.11 ppm	Amoore and Hautala 1983
Air	0.16 ppm	Amoore and Hautala 1983
Taste threshold	No data	
Solubility:		
Water at 25°C	2.12x10^5 mg/L	Seidell 1941
Organic solvents	Miscible with lower alcohols, ketones, benzene, diethyl ether, and other common organic solvents	Tomlin 2003
Partition coefficients:		
Log K_{ow}	-0.01	Hansch and Leo 1995
K_{oc}	24 (estimated)[a]	Lyman 1982
Vapor pressure at 25°C	274 mmHg	Daubert and Danner 1987
Henry's law constant at 25°C	1.22x10^{-4} atm-m^3/mol	Gaffney et al. 1987
Autoignition temperature	220 °C	NLM 2024
Flashpoint	-18 °C (open cup) -26 °C (closed cup)	NLM 2024; O'Neil 2013
Flammability limits	2.8–31 volume %	NLM 2024
Conversion factors		
Air	1 ppm (v/v)=2.3 mg/m^3 1 mg/m^3=0.43 ppm (v/v)	Verschueren 2001

[a]K_{oc} value was estimated using the measured log K_{ow} (-0.01) and a linear regression equation described in Lyman (1982).