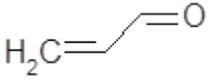


## CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

### 4.1 CHEMICAL IDENTITY

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 2023; RTECS 2019
Chemical formula	C <sub>3</sub> H <sub>4</sub> O	NLM 2023
SMILES	C=CC=O	NLM 2023
Chemical structure		
CAS Registry Number	107-02-8	NLM 2023

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

### 4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding physical and chemical properties of acrolein is presented in Table 4-2.

## 4. CHEMICAL AND PHYSICAL INFORMATION

**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 2023
Boiling point	52.3 °C	NLM 2023
Density at 20°C	0.840 g/cm <sup>3</sup>	NLM 2023
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 <sup>5</sup> 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 <sub>ow</sub>	-0.01	Hansch and Leo 1995
K <sub>oc</sub>	24 (estimated) <sup>a</sup>	Lyman 1982
Vapor pressure at 25°C	274 mmHg	Daubert and Danner 1987
Henry's law constant at 25°C	1.22x10 <sup>-4</sup> atm-m <sup>3</sup> /mol	Gaffney et al. 1987
Autoignition temperature	220 °C	NLM 2023
Flashpoint	-18 °C (open cup) -26 °C (closed cup)	NLM 2023; O'Neil 2013
Flammability limits	2.8–31 volume %	NLM 2023
Conversion factors		
Air	1 ppm (v/v)=2.3 mg/m <sup>3</sup> 1 mg/m <sup>3</sup> =0.43 ppm (v/v)	Verschueren 2001

<sup>a</sup>K<sub>oc</sub> value was estimated using the measured log K<sub>ow</sub> (-0.01) and a linear regression equation described in Lyman (1982).