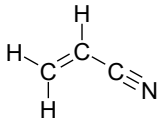
CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of acrylonitrile is presented in Table 4-1.

Table 4-1. Chemical Identity of Acrylonitrile

Characteristic	Information
Chemical name	Acrylonitrile
Synonym(s) and registered trade name(s)	Cyanoethylene; 2-Propenenitrile; Vinyl cyanide; Acritet, Caswell No. 010; ENT 54; Fumigrain; Ventox
Chemical formula	C_3H_3N
SMILES	C=CC#N
Chemical structure	
CAS Registry Number	107-13-1

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

Source: NLM 2022

4.2 PHYSICAL AND CHEMICAL PROPERTIES

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

Table 4-2. Physical and Chemical Properties of Acrylonitrile

Property	Information	Reference
Molecular weight	53.06	Weast 1985
Color	Colorless	Verschueren 1983
Physical state	Liquid	Verschueren 1983
Melting point	-83°C	Verschueren 1983
Boiling point	77.4°C	Verschueren 1983
Density at 20°C	0.8060	Verschueren 1983
Odor	Pungent (onion, garlic)	Verschueren 1983
Odor threshold:		
Water	18.6 mg/L	Verschueren 1983
Air	47 mg/m^3	Verschueren 1983

Table 4-2. Physical and Chemical Properties of Acrylonitrile

Property	Information	Reference
Solubility:		
Water at 20°C	79,000 mg/L 6,803 mg/L	Klein et al. 1957 Yalkowsky et al. 2010
Organic solvents	Soluble in all common organic solvents	Sax and Lewis 1987
Partition coefficients:		
Log K_{ow}	0.25	EPA 1982a
Log K_{oc}	1.00 and 1.10 -0.07 (estimated from Log K_{ow})	EPA 1992 EPA 1982a
Vapor pressure at 22.8°C at 25°C	 100 mm Hg 109 mm Hg	 EPA 1982a NLM 2022
Henry's law constant at 25°C	1.18×10^{-5} atm-m^3/mol 8.8×10^{-5} atm-m^3/mol (calculated from vapor pressure/water solubility)	Sander 2015 EPA 1982a
Autoignition temperature	481°C	Sax 1984
Flashpoint	-1°C	Sax 1984
Explosive limits	3–17%	Sax and Lewis 1987
Conversion factors	1 ppm=2.203 mg/m^3 1 mg/m^3=0.454 ppm	Verschueren 1983