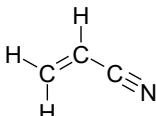


CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Data pertaining to the chemical identity of acrylonitrile are listed 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 ₃ H ₃ N
Chemical structure	
CAS Registry Number	107-13-1

CAS = Chemical Abstracts Service

Source: NLM 2022

4.2 PHYSICAL AND CHEMICAL PROPERTIES

The physical and chemical properties of acrylonitrile are 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

4. CHEMICAL AND PHYSICAL INFORMATION

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	100 mm Hg	EPA 1982a
at 25°C	109 mm Hg	NLM 2022
Henry's law constant at 25°C		
	1.18x10 ⁻⁵ atm-m ³ /mol 8.8x10 ⁻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