

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Table 3-1 lists common synonyms, trade names and other pertinent identification information for acrylonitrile.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Table 3-2 lists important physical and chemical properties of acrylonitrile.

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TABLE 3-1. Chemical Identity of Acrylonitrile

	Value	Reference
Chemical name	Acrylonitrile	NLM 1988
Synonyms	Cyanoethylene; 2-propenenitrile; vinyl cyanide	NLM 1988
Trade names	Acritet, Caswell No. 010, ENT 54, Fumigrain, Ventox	HSDB 1988; Windholz 1983
Chemical formula	C ₃ H ₃ N	NLM 1988
Chemical structure		
Identification numbers:		
CAS registry	107-13-1	NLM 1988
NIOSH RTECS	AT5250000	NIOSH 1981, 1982
EPA Hazardous Waste	U009	NLM 1988
OHM/TADS	7216574	HSDB 1988
DOT/UN/NA/IMCO	UN1093	NLM 1988
Shipping	IMCO 3.2	HSDB 1988
HSDB	176	NLM 1988
NCI	C50215	NLM 1988

CAS = Chemical Abstracts Service; NIOSH = National Institute for Occupational Safety and Health; RTECS = Registry of Toxic Effects of Chemical Substances; EPA = Environmental Protection Agency; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute.

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TABLE 3-2. Physical and Chemical Properties of Acrylonitrile

Property	Value	Reference
Molecular weight	53.06	Weast 1985
Color	Colorless	Verschuieren 1983
Physical state	Liquid	Verschuieren 1983
Melting point	-83°C	Verschuieren 1983
Boiling point	77.4°C	Verschuieren 1983
Density at 20°C	0.8060	Weast 1985
Odor	Pungent (onion, garlic)	Verschuieren 1983
Odor threshold:		
Water	18.6 mg/L	Verschuieren 1983
Air	47 mg/m ³	Verschuieren 1983
Solubility:		
Water at 20°C	79,000 mg/L	Klein et al. 1957
Organic solvents	Soluble in all common organic solvents	Sax and Lewis 1987
Partition coefficients:		
Log octanol/water	-0.92	Verschuieren 1983
Log K _{oc}	-0.07	Mabey et al. 1982
Vapor pressure at 22.8°C	100 mmHg	Mabey et al. 1982
Henry's law constant:	8.8x10 ⁻⁵ atm-m ³ /mol	Mabey et al. 1982
Autoignition temperature	481°C	Sax 1984
Flashpoint (closed cup)	-1°C	Sax 1984
Flammability limits	3% to 17%	Sax and Lewis 1987
Conversion factors	1 ppm = 2.203 mg/m ³ 1 mg/m ³ =0.454 ppm	Verschuieren 1983

