

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Data pertaining to the chemical identity of acrolein are listed in Table 3-1.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

The physical and chemical properties of acrolein are presented in Table 3-2.

3. CHEMICAL AND PHYSICAL INFORMATION

TABLE 3-1. Chemical Identity of Acrolein

	Value	Reference
Chemical name	Acrolein	
Synonyms	Acraldehyde acrylaldehyde allyl aldehyde 2-propenal propylene aldehyde	SANSS 1988
Trade names	Aqualin, MAGNACIDE H®	Bennett 1981, 1982
Chemical formula	C ₃ H ₄ O	CAS 1988
Chemical structure	$\text{CH}_2 = \text{CH - CHO}$	SANSS 1988
Identification numbers:		
CAS Registry	107-02-8	CAS 1988
NIOSH RTECS	AS1050000	RTECS 1988
EPA Hazardous Waste	P003	HSDB 1988
OHM-TADS	7216793	OHM-TADS 1988
DOT/UN/NA/IMCO	UN 1092	HSDB 1988
IMCO	3.1	HSDB 1988
HSDB	177	HSDB 1988
NCI	Not available	

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

3. CHEMICAL AND PHYSICAL INFORMATION

TABLE 3-2. Physical and Chemical Properties of Acrolein

Property	Value	Reference
Molecular weight	56.06	Hess et al. 1978
Color	Colorless or yellowish	Hess et al. 1978
Physical State	Liquid	Hess et al. 1978
Melting point	-86.9°C	Weast 1983
Boiling point	52.5-53.5°C	Weast 1983
Density at 20°C	0.8389 g/m ³	Riddick et al. 1986
Specific gravity, 20/4°C	0.8410	Weast 1983
Odor	Disagreeable, choking odor, pungent	Hawley 1981; Windholz 1983
Odor threshold:		
Water	0.11 ppm	Amoore and Hautala 1983
Air	0.16 ppm	
Solubility:		
Water at 20°C	206,000 mg/L	Hess et al. 1978
Organic solvents	Miscible with lower alcohols, ethers, hydrocarbons, acetone, benzene	Tweedy and Houseworth 1976
Partition coefficients:		
Log octanol/water	-0.01	Hansch and Leo 1985
Log K _{oc}	51-270	Irwin 1988
Vapor pressure at 20°C:	220 mmHg	Hess et al. 1978
Henry's law constant:		
at 20°C	3.06 x 10 ⁻⁵ atm·m ³ /mol	Snider and Dawson 1985
Autoignition temperature	234°C	Hess et al. 1978
Flashpoint	-18°C (open cup) -26°C (closed cup)	Hess et al. 1978
Flammability limits in air	2.8-31 volume %	Hess et al. 1978
Conversion factors:		
ppm (v/v) to mg/m ³ in air at 25°C	1 ppm (v/v) = 2.29 mg/m ³	
mg/m ³ to ppm (v/v) in air at 25°C	1 mg/m ³ = 0.44 ppm (v/v)	

