

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

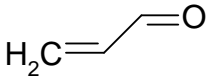
Data pertaining to the chemical identity of acrolein are listed in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

The physical and chemical properties of acrolein are presented in Table 4-2.

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Table 4-1. Chemical Identity of Acrolein

Characteristic	Information	Reference
Synonyms	Acraldehyde, acrylic aldehyde, acrylaldehyde, allyl aldehyde, ethylene aldehyde, 2-propenal, propylene aldehyde	HSDB 2007; RTECS 2007
Trade name	Aqualin, Biocide, Crolean, MAGNACIDE B [®] , MAGNACIDE H [®] , Slimicide	RTECS 2007
Chemical formula	C ₃ H ₄ O	HSDB 2007
Chemical structure		
Identification numbers:		
CAS registry	107-02-8	HSDB 2007
NIOSH RTECS	AS1050000	RTECS 2007
EPA hazardous waste	P003	HSDB 2007
OHM/TADS	7216793	OHM/TADS 1988
DOT/UN/NA/IMDG shipping	UN 1092	HSDB 2007
IMCO	3.1	HSDB 2007
HSDB	177	HSDB 2007
NCI	Not available	

CAS = Chemical Abstracts Services; DOT/UN/NA/IMDG = Department of Transportation/United Nations/North America/Intergovernmental Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances 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

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Table 4-2. Physical and Chemical Properties of Acrolein

Property	Information	Reference
Molecular weight	56.06	O'Neil 2001
Color	Colorless or yellowish	Lewis 1997
Physical state	Liquid	Lewis 1997
Melting point	-87.7 °C	Lide 2000
Boiling point	52.6 °C	Lide 2000
Density at 20 °C	0.840 g/cm ³	Lide 2000
Odor	Disagreeable, choking odor, pungent	Lewis 1997; O'Neil 2001
Odor threshold:		
Water	0.11 ppm	Amoore and Hautala 1983
Air	0.16 ppm	Amoore and Hautala 1983
Solubility:		
Water at 25 °C	2.12x10 ⁵ 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 _{ow}	-0.01	Hansch and Leo 1995
K _{oc}	24 (estimated) ^a	Lyman 1982
Vapor pressure at 25 °C	274 mmHg	Daubert and Danner 1987
Henry's law constant at 25 °C	1.22x10 ⁻⁴ atm·m ³ /mol	Gaffney et al. 1987
Autoignition temperature	220 °C	HSDB 2007
Flashpoint	-18 °C (open cup) -26 °C (closed cup)	HSDB 2007; O'Neil 2001
Flammability limits	2.8–31 volume %	HSDB 2007
Conversion factors		
Air	1 ppm (v/v)=2.328 mg/m ³ 1 mg/m ³ =0.43 ppm (v/v)	Verschueren 2001

^aK_{oc} value was estimated using the measured log K_{ow} (-0.01) and a linear regression equation described in Lyman (1982).