3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

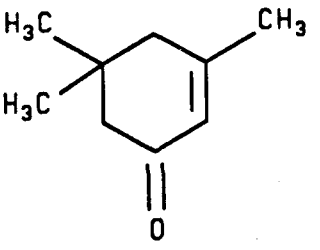
Data pertaining to the chemical identity of isophorone are listed in Table 3-l.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

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

3. CHEMICAL AND PHYSICAL INFORMATION

TABLE 3-1. Chemical Identity of Isophorone

	Value	Reference
Chemical Name	2-Cyclohexen-1-one, 3,5,5-trimethyl-	CAS 1988
Synonyms	Isoacetophorone Isoforon 1,5,5-Trimethyl-3-oxocyclohexene	CAS 1988; SANSS 1988
Trade Name(s)	No data	
Chemical Formula	$C_9 H_{14} O$	CAS 1988
Chemical Structure		SANSS 1988
Identification Numbers:		
CAS Registry	78-59-1	CAS 1988
NIOSH RTECS	GW7700000	RTECS 1988
EPA Hazardous Waste	No data	
OHM-TADS	7216766	OHM-TADS 1988
DOT/UN/NA/IMCO	No data	
HSDB	619	HSDB 1988
NCI	C55618	HSDB 1988

CAS = Chemical Abstracts Service
NIOSH = National Institute for Occupational Safety and Health
RTECS = Registry of Toxic Effects of Chemical Substances
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

TABLE 3-2. Physical and Chemical Properties of Isophorone

Property	Value	Reference
Molecular weight	138.21	Union Carbide 1968
Color	Water-white	Hawley 1981
Physical state	Liquid	Hawley 1981
Freezing point	-8.1°C	Union Carbide 1968
Boiling point	215.3°C	Union Carbide 1968
Specific gravity, 20/20°C	0.9229	Union Carbide 1968
Odor	Mild	Union Carbide 1968
Odor threshold		
Water	5.4 ppm (w/v)	Amoore and Hautala 1983
Air	0.20 ppm (v/v)	Amoore and Hautala 1983
Solubility		
Water	12,000 mg/L (20°C) 14,500 mg/L (25°C)	Union Carbide 1968 Veith et al. 1980
Organic Solvents	Soluble in ether, acetone, alcohol	Weast 1985
Partition coefficients		
Log octanol/water	1.67 (20°C) (Experimental)	Veith et al. 1980
Log K_{oc}	No data	
Vapor pressure	0.3 mm Hg (20°C)	Extrapolated using data from Union Carbide 1968
Henry's Law constant	4.55×10^{-6} atm-m^3/mol (20°C)	Calculated from vapor pressure and water solubility data
Autoignition temperature	864°F (462°C)	Hawley 1981
Flashpoint, open cup	184°F (84°C)	Dean 1985
Flammability limits	0.8-3.5 vol %	HSDB 1988
Conversion factors		
ppm (v/v) to mg/m^3 in air (20°C)	ppm (v/v) x 5.75 = mg/m^3	
mg/m^3 to ppm (v/v) in air (20°C)	mg/m^3 x 0.174 = ppm (v/v)	