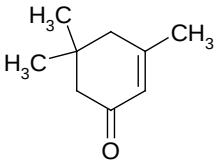
CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Table 4-1 lists common synonyms, trade names and other pertinent identification information for isophorone.

Table 4-1. Chemical Identity of Isophorone

Characteristic	Information	Reference
Chemical name	2-Cyclohexen-1-one,3,5,5-trimethyl-	CAS 1988
Synonym(s) and registered trade name(s)	Isophorone; Isoacetophorone; 1,5,5-Trimethyl-3-oxocyclohexene	CAS 1988; SANSS 1988
Chemical formula	$C_9H_{14}O$	CAS 1988
Chemical structure		SANSS 1988
CAS Registry Number	78-59-1	CAS 1988

CAS = Chemical Abstracts Service

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Table 4-2 lists important physical and chemical properties of isophorone.

Table 4-2. Physical and Chemical Properties of Isophorone

Property	Information	Reference
Molecular weight	138.1	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
Density at 20°C	0.9229 g/m^3	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 at 20°C	12,000 mg/L	Union Carbide 1968
Organic solvents	Soluble in ether, acetone, alcohol	Weast 1985
Partition coefficients:		
Log K_{ow}	1.67 (20°C, experimental)	Veith et al. 1980
Log K_{oc}	No data	
Vapor pressure at 20°C	0.3 mmHg	Extrapolated using data from Union Carbide 1968
Henry's law constant at 20°C	$4.55x10^{-6}$ atm-m^3/mol	Calculated from vapor pressure and water solubility data
Autoignition temperature	864°F (462°C)	Hawley 1981
Flashpoint	184°F (84°C) (open cup)	Dean 1985
Flammability limits	0.8–3.5 vol%	HSDB 1988
Conversion factors (in air, 20°C)	ppm (v/v)x5.75=mg/m^3	
	mg/m^3x0.174=ppm (v/v)	