

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

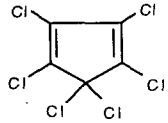
Hexachlorocyclopentadiene (HCCPD) is a yellow to yellow-green dense oily liquid with a pungent odor. It is used as an intermediate in the manufacture of pesticides, flame-retardant materials, and some plastics. Information regarding the chemical identity of HCCPD is located in Table 3- 1.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

HCCPD is slightly soluble in water and will react slowly with water to form hydrochloric acid (HSDB 1998). It is a corrosive chemical, and contact can burn the eyes and skin. While HCCPD itself does not burn, it may decompose upon heating to produce toxic fumes (HSDB 1998). Information regarding the physical and chemical properties of HCCPD is located in Table 3-2.

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Table 3-1. Chemical Identity of HCCPD

Characteristic	Information	Reference
Chemical name	Hexachlorocyclopentadiene	HSDB 1998
Synonym(s)	HCCPD; 1,3-cyclopentadiene; 1,2,3,4,5,5-hexachloro-; hex; perchlorocyclopentadiene	HSDB 1998
Registered trade name(s)	C-56; graphlox; HRS 1655	
Chemical formula	C ₅ Cl ₆	HSDB 1998
Chemical structure		Verschueren 1983
Identification numbers:		
CAS registry	77-47-4	HSDB 1998
NIOSH RTECS	GY1225000	HSDB 1998
EPA hazardous waste	U130	HSDB 1998
OHM/TADS	7800117	HSDB 1998
DOT/UN/NA/IMCO shipping	UN2646 IMCO 6.1	HSDB 1998
HSDB	4011	HSDB 1998
NCI	C55607	HSDB 1998

CAS = Chemical Abstracts Service; DOT/UN/NA/IMO = Dept. of Transportation/United Nations/ North America/International 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 3-2. Physical and Chemical Properties of HCCPD

Property	Information	Reference
Molecular weight	272.77	Weast 1989
Color	Lemon yellow/yellow-green	EPA 1991a
Physical state	Liquid	EPA 1991a
Melting point	-9 °C	Weast 1989
Boiling point at 753 mm Hg	239 °C	Weast 1989
Density at 25 °C	1.7019 g/mL	Weast 1989
Odor	Pungent	EPA 1991a
Odor threshold:		
Water	0.0014–0.0074 mg/L	Amoore and Hautala 1983; Verschuereen 1983
Air	0.03 ppm (0.34 mg/m ³) 1.5–3.3 mg/m ³	Amoore and Hautala 1983 Ruth 1986
Solubility:		
Water at 25 °C	2.1 mg/L 1.03–1.25 mg/L	EPA 1991a WHO 1991
Organic solvents	Miscible in acetone carbon tetrachloride, methanol, hexane	ACGIH 1992
Partition coefficients:		
Log K _{ow}	4.0–5.04	Mabey et al 1982; Wolfe et al. 1982
Log K _{oc}	3.68–4.08	Mabey et al. 1982; Wolfe et al. 1982
Vapor pressure at 25 °C	0.08 mm Hg	Verschuereen 1983
Henry's law constant at 24.8 °C	2.7x10 ⁻² atm·m ³ /mol	Wolfe et al. 1982
Autoignition temperature	No data	
Flashpoint	No data	
Flammability limits	No data	
Conversion factors:	1 ppm = 11.3 mg/m ³ ; 1 mg/m ³ = 0.088 ppm	WHO 1991
Explosive limits	No data	

