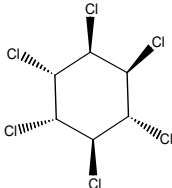
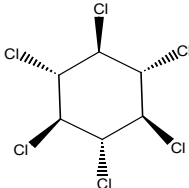


## CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

### 4.1 CHEMICAL IDENTITY

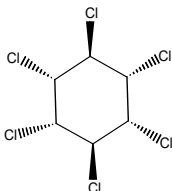
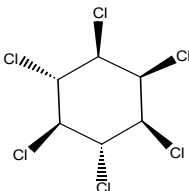
HCH consists of eight isomers (Safe 1993). Only  $\gamma$ -HCH,  $\alpha$ -HCH,  $\beta$ -HCH, and  $\delta$ -HCH are of commercial significance and considered in this profile. The pesticide lindane refers to products that contain >99%  $\gamma$ -HCH. The  $\alpha$ -,  $\beta$ -, and  $\delta$ -isomers, as well as technical-grade HCH are not synonymous with  $\gamma$ -HCH (Farm Chemicals Handbook 1993). Technical-grade HCH (CAS Registry Number 608-73-1) is not an isomer of HCH, but rather a mixture of several isomers; it consists of approximately 60–70%  $\alpha$ -HCH, 5–12%  $\beta$ -HCH, 10–15%  $\gamma$ -HCH, 6–10%  $\delta$ -HCH, and 3–4%  $\epsilon$ -HCH (Kutz et al. 1991). Information regarding the chemical identities of  $\alpha$ -,  $\beta$ -,  $\gamma$ -, and  $\delta$ -HCH is located in Table 4-1.

**Table 4-1. Chemical Identity of Hexachlorocyclohexane Isomers<sup>a</sup>**

Characteristic	$\alpha$ -Hexachlorocyclohexane	$\beta$ -Hexachlorocyclohexane
Synonym(s) and registered trade name(s)	1-alpha, 2-alpha, 3-beta, 4-alpha, 5-beta, 6-beta-benzene-trans-hexachloride; alpha-1,2,3,4,5,6-hexachlorocyclohexane; alpha-benzene hexachloride; alpha-BHC; alpha-HCH; alpha-hexachloran; alpha-hexachlorane; alpha-hexachlorocyclohexane; alpha-lindane; benzenehexachloride-alpha-isomer; cyclohexane 1,2,3,4,5,6-(alpha, DL); cyclohexane 1,2,3,4,5,6-hexachloro, alpha-; cyclohexane 1,2,3,4,5,6-hexachloro-, alpha-isomer; cyclohexane, alpha-1,2,3,4,5,6-hexachloro; ENT 9232	1-alpha, 2-beta, 3-alpha, 4-beta, 5-alpha, 6-beta-hexachlorocyclohexane; beta 1,2,3,4,5,6-hexachlorocyclohexane; beta-benzenehexachloride; beta-BHC; beta HCH; beta-hexachloran; beta-hexachlorobenzene; beta-lindane; cyclohexane, 1,2,3,4,5,6-hexachloro-, beta-; cyclohexane, 1,2,3,4,5,6-hexachloro-, beta-isomer; cyclohexane, 1,2,3,4,5,6-hexachloro-, trans-; cyclohexane, beta-1,2,3,4,5,6-hexachloro-; ENT 9233; trans-alpha-benzenehexachloride
Chemical formula	C <sub>6</sub> H <sub>6</sub> Cl <sub>6</sub>	C <sub>6</sub> H <sub>6</sub> Cl <sub>6</sub>
Chemical structure		
CAS Registry Number	319-84-6	319-85-7

## 4. CHEMICAL AND PHYSICAL INFORMATION

**Table 4-1. Chemical Identity of Hexachlorocyclohexane Isomers<sup>a</sup>**

Characteristic	$\gamma$ -Hexachlorocyclohexane	$\delta$ -Hexachlorocyclohexane
Synonym(s) and registered trade name(s)	Lindane; 1-alpha, 2-alpha, 3-beta, 4-alpha, 5-alpha, 6-beta-hexachlorocyclohexane; benzene hexachloride-gamma-isomer; BHC; cyclohexane 1,2,3,4,5,6-hexachloro-gamma-isomer; ENT 7796; gamma-benzene hexachloride; gamma-BHC; gamma-hexachlorocyclohexane; gamma-1,2,3,4,5,6-hexachlorocyclohexane; gamma-HCH; gamma-lindane; HCH; HCCH; hexachlorocyclohexane, gamma-isomer; 1,2,3,4,5,6-hexachlorocyclohexane, gamma-isomer, Etan 3G (Diachem S.P.A.); Forlin; Gamaphex; Isotox (Chevron Chemical Co.); Germate Plus (Gustafson Inc.); Gamma-Mean 400 and Gamma Mean L. (Oregon-California Chemicals, Inc.); Hammer (Exsin Industries); Lindagam; Novigam; Silvanol; Kwell	1-alpha,2-alpha,3-alpha, 4-beta, 5-alpha, 6-beta-hexachlorocyclohexane; cyclohexane, 1,2,3,4,5,6-hexachloro-, delta-isomer; cyclohexane, delta-1,2,3,4,5,6-hexachloro-; delta-(AEEEE)-1,2,3,4,5,6-hexachlorocyclohexane; delta-benzenehexachloride; delta-BHC; delta-HCH; delta-1,2,3,4,5,6-hexachlorocyclohexane; delta-lindane; ENT 9234
Chemical formula	$C_6H_6Cl_6$	$C_6H_6Cl_6$
Chemical structure		
CAS Registry Number	58-89-9	319-86-8

<sup>a</sup>All information obtained from NLM 2021.

CAS = Chemical Abstracts Service

**4.2 PHYSICAL AND CHEMICAL PROPERTIES**

Information regarding the physical and chemical properties of  $\alpha$ -,  $\beta$ -,  $\gamma$ -, and  $\delta$ -HCH is located in Table 4-2.

## 4. CHEMICAL AND PHYSICAL INFORMATION

**Table 4-2. Physical and Chemical Properties of Hexachlorocyclohexane Isomers**

Property	$\alpha$ -Hexachloro- cyclohexane (CAS 319-84-6)	$\beta$ -Hexachloro- cyclohexane (CAS 319-85-7)	$\gamma$ -Hexachlorocyclo- hexane (CAS 58-89-9)	$\delta$ -Hexachloro- cyclohexane (CAS 319-86-8)
Molecular weight	290.83 <sup>a</sup>	290.83 <sup>a</sup>	290.83 <sup>a</sup>	290.83 <sup>a</sup>
Color	Brownish to white <sup>b</sup>	No data	White <sup>c</sup>	No data
Physical state	Crystalline solid <sup>b</sup> ; monoclinic prisms <sup>a</sup>	Crystalline solid <sup>a,d</sup>	Crystalline solid <sup>d</sup> ; monoclinic prisms <sup>b</sup>	Fine plates <sup>a,c</sup>
Melting point	159–160°C <sup>a</sup>	314–315°C <sup>a</sup>	112.5°C <sup>a,e</sup>	141–142°C <sup>a</sup>
Boiling point	288°C at 760 mmHg <sup>b</sup>	60°C at 0.5 mmHg <sup>a</sup>	323.4°C at 760 mmHg <sup>b</sup>	60°C at 0.36 mmHg <sup>a</sup>
Density (g/cm <sup>3</sup> )	1.87 at 20°C <sup>a</sup>	1.89 at 19°C <sup>a</sup>	1.89 at 19°C <sup>f</sup>	No data
Odor	Phosgene-like odor <sup>b</sup>	No data	Slightly musty odor <sup>b</sup>	No data
Odor threshold:				
Water	0.88 ppm for unspecified purity <sup>g</sup>	0.00032 mg/kg <sup>h</sup>	12 mg/kg <sup>h</sup>	No data
Air	No data	No data	No data	No data
Solubility:				
Water	10 ppm <sup>i</sup> ; 69.5 mg/L at 28°C <sup>j</sup>	5 ppm <sup>k</sup>	17 ppm <sup>k</sup> ; 7.3 mg/L at 25°C <sup>b</sup>	10 ppm <sup>i</sup>
Organic solvents	Soluble in alcohol <sup>l</sup> ; 1.8 g/100 g in ethanol <sup>l</sup> ; 6.2 g/100 g in ether <sup>j</sup>	1.1 g/100 g in ethanol; 1.8 g/100 g in ether; 1.9 g/100 g in benzene <sup>i</sup>	6.4 g/100 g in ethanol; 20.8 g/100 g in ether; 28.9 g/100 g in benzene <sup>i</sup>	24.4 g/100 g in ethanol; 35.4 g/100 g in ether; 41.4 g/100 g in benzene <sup>i</sup>
Partition coefficients:				
Log K <sub>ow</sub>	3.8 <sup>l</sup>	3.78 <sup>l</sup>	3.72 <sup>l</sup>	4.14 <sup>l</sup>
Log K <sub>oc</sub>	3.57 <sup>f</sup>	3.57 <sup>m</sup>	3.0 <sup>m</sup> ; 3.57 <sup>f</sup>	3.8 <sup>f</sup>
Vapor pressure	4.5x10 <sup>-5</sup> mmHg at 25°C <sup>b</sup>	3.6x10 <sup>-7</sup> mmHg at 20°C <sup>b</sup>	4.2x10 <sup>-5</sup> mmHg at 20°C <sup>b</sup> ; 9.4x10 <sup>-6</sup> mmHg at 20°C <sup>b</sup>	3.5x10 <sup>-5</sup> mmHg at 25°C <sup>b</sup>
Henry's law constant	6.86x10 <sup>-6b</sup>	4.5x10 <sup>-7m,n</sup>	3.5x10 <sup>-6b</sup>	2.1x10 <sup>-7o,p</sup>
Autoignition temperature	No data	No data	Not flammable <sup>b</sup>	No data
Flashpoint	No data	No data	Approximately 150°F (closed cup) <sup>b</sup>	No data

## 4. CHEMICAL AND PHYSICAL INFORMATION

**Table 4-2. Physical and Chemical Properties of Hexachlorocyclohexane Isomers**

Property	$\alpha$ -Hexachloro- cyclohexane (CAS 319-84-6)	$\beta$ -Hexachloro- cyclohexane (CAS 319-85-7)	$\gamma$ -Hexachlorocyclo- hexane (CAS 58-89-9)	$\delta$ -Hexachloro- cyclohexane (CAS 319-86-8)
Flammability limits	No data	No data	Not flammable <sup>b</sup>	No data
Conversion factors <sup>q</sup>	ppm to mg/m <sup>3</sup> in air (20°C): ppm x 4.96 = mg/m <sup>3</sup> ; mg/m <sup>3</sup> to ppm in air (20°C): mg/m <sup>3</sup> x 0.20 = ppm			
Explosive limits	No data	No data	No data	No data

CAS = Chemical Abstracts Service

<sup>a</sup>Lide 1991.

<sup>b</sup>NLM 2021.

<sup>c</sup>Kirk and Othmer 1985.

<sup>d</sup>IARC 1979.

<sup>e</sup>Budavari et al. 1989.

<sup>f</sup>Weiss 1986.

<sup>g</sup>Fazzalari 1978.

<sup>h</sup>Verschueren 1983.

<sup>i</sup>Clayton and Clayton 1981.

<sup>j</sup>Kurihara et al. 1973.

<sup>k</sup>Hollifield 1979.

<sup>l</sup>Hansch and Leo 1995.

<sup>m</sup>Rippen et al. 1982.

<sup>n</sup>Veith et al. 1979.

<sup>o</sup>Pankow et al. 1984.

<sup>p</sup>EPA 1982a.

<sup>q</sup>Same for all isomers.