CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

HCH consists of eight isomers (Safe 1993). Only γ-HCH, α-HCH, β-HCH, and δ-HCH are of commercial significance and considered in this profile. The pesticide lindane refers to products that contain >99% γ-HCH. The α-, β-, and δ-isomers, as well as technical-grade HCH are not synonymous with γ-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% α-HCH, 5–12% β-HCH, 10–15% γ-HCH, 6–10% δ-HCH, and 3–4% ε-HCH (Kutz et al. 1991). Information regarding the chemical identities of α-, β-, γ-, and δ-HCH is located in Table 4-1.

Table 4-1. Chemical Identity of Hexachlorocyclohexane Isomers[a]

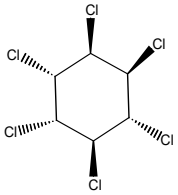
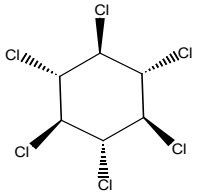
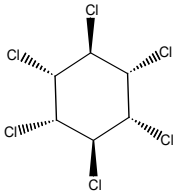
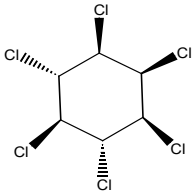
Characteristic	α-Hexachlorocyclohexane	β-Hexachlorocyclohexane
Synonym(s) and registered trade name(s)	1-alpha, 2-alpha, 3-beta, 4-alpha, 5-beta, 6-beta-benzene-trans-hexachloride; alpha-1,2,3,4,5,6-hexachlorocyclohexane; alpha-benzene hexachloride; alpha-BHC; alpha-HCH; alpha-hexachloran; alpha-hexachlorane; 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-aplha, 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	$C_6H_6Cl_6$	$C_6H_6Cl_6$
SMILES	C1(C(C(C(C(C1Cl)Cl)Cl)Cl)Cl)Cl	C1(C(C(C(C(C1Cl)Cl)Cl)Cl)Cl)Cl
Chemical structure		
CAS Registry Number	319-84-6	319-85-7

Table 4-1. Chemical Identity of Hexachlorocyclohexane Isomers[a]

Characteristic	γ-Hexachlorocyclohexane	δ-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-(AEEEEE)- 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	$C_6H_6Cl_6$	$C_6H_6Cl_6$
SMILES	C1(C(C(C(C(C1Cl)Cl)Cl)Cl)Cl)Cl	C1(C(C(C(C(C1Cl)Cl)Cl)Cl)Cl)Cl
Chemical structure		
CAS Registry Number	58-89-9	319-86-8

[a]All information obtained from NLM 2021.

CAS = Chemical Abstracts Service; SMILES = Simplified molecular-input line-entry system

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of α-, β-, γ-, and δ-HCH is located in Table 4-2.

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

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

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

Property	α-Hexachloro-cyclohexane (CAS 319-84-6)	β-Hexachloro-cyclohexane (CAS 319-85-7)	γ-Hexachlorocyclo-hexane (CAS 58-89-9)	δ-Hexachloro-cyclohexane (CAS 319-86-8)
Flammability limits	No data	No data	Not flammable[b]	No data
Conversion factors[q]	ppm to mg/m^3 in air (20°C): ppm x 4.96 = mg/m^3; mg/m^3 to ppm in air (20°C): mg/m^3 x 0.20 = ppm			
Explosive limits	No data	No data	No data	No data

CAS = Chemical Abstracts Service

[a]Lide 1991.
[b]NLM 2021.
[c]Kirk and Othmer 1985.
[d]IARC 1979.
[e]Budavari et al. 1989.
[f]Weiss 1986.
[g]Fazzalari 1978.
[h]Verschueren 1983.
[i]Clayton and Clayton 1981.
[j]Kurihara et al. 1973.
[k]Hollifield 1979.
[l]Hansch and Leo 1995.
[m]Rippen et al. 1982.
[n]Veith et al. 1979.
[o]Pankow et al. 1984.
[p]EPA 1982a.
[q]Same for all isomers.