

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

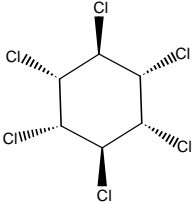
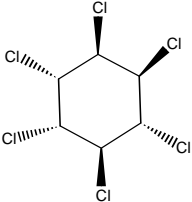
HCH consists of eight isomers (Safe 1993). Only γ -HCH, α -HCH, β -HCH, and δ -HCH are of commercial significance and considered in this profile. The pesticide lindane refers to products that contain >99% γ -HCH. The α -, β -, and δ -isomers, as well as technical-grade HCH are not synonymous with γ -HCH (Farm Chemicals Handbook 1993). Technical-grade HCH 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 γ -HCH, α -HCH, β -HCH, and δ -HCH is located in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

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

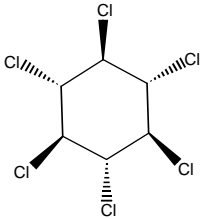
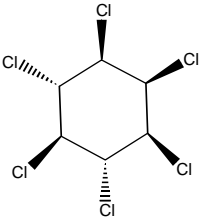
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Table 4-1. Chemical Identity of Hexachlorocyclohexane Isomers^a

| Characteristic | γ -hexachlorocyclohexane | α -hexachlorocyclohexane |
|--------------------------|---|--|
| Synonym(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 ^b | 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 ^b |
| Registered trade name(s) | 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 ^c ; Kwell (pharmaceutical shampoo/lotion) ^d | No data |
| Chemical formula | $C_6H_6Cl_6$ | $C_6H_6Cl_6$ ^b |
| Chemical structure |  |  |
| Identification numbers: | | |
| CAS registry | 58-89-9 | 319-84-6 |
| NIOSH RTECS | GV4900000 | GV3500000 |
| EPA hazardous waste | U129; D013 | No data |
| OHM/TADS | 7216531 | 810002 |
| DOT/UN/NA/IMCO shipping | NA 2761 lindane; IMCO 6.1 lindane; UN 2761, organochlorine pesticides, solid toxic, not otherwise specified | No data |
| HSDB | 646 | 6029 |
| NCI | C00204 | No data |

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Table 4-1. Chemical Identity of Hexachlorocyclohexane Isomers^a

| Characteristic | β -hexachlorocyclohexane | δ -hexachlorocyclohexane |
|--------------------------|--|---|
| Synonym(s) | 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 ^b | 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 ^b |
| Registered trade name(s) | No data | No data |
| Chemical formula | C ₆ H ₆ Cl ₆ | C ₆ H ₆ Cl ₆ |
| Chemical structure |  |  |
| Identification numbers: | | |
| CAS registry | 319-85-7 | 319-86-8 |
| NIOSH RTECS | GV4375000 | GV4550000 |
| EPA hazardous waste | No data | No data |
| OHM/TADS | No data | No data |
| DOT/UN/NA/IMCO shipping | No data | No data |
| HSDB | 6183 | 6184 |
| NCI | No data | No data |

^aAll information obtained from HSDB 1997 except where noted.

^bRTECS 1993

^cFarm Chemicals Handbook 1993

^dBudavari et al. 1989

CAS = Chemical Abstracts Service; DOT/UN/NA/IMCO = Department 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 4-2. Physical and Chemical Properties of Hexachlorocyclohexane Isomers

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

^aLide 1991^bKirk-Othmer 1985^cHSDB 2003^dIARC 1979^eBudavari et al. 1989^fWeiss 1986^gVerschuereen 1983^hFazzalari 1978ⁱHollifield 1979^jClayton and Clayton 1981^kKuihara et al. 1973^lHansch and Leo 1995^mRipping 1972ⁿVeith et al. 1979^oPankow et al. 1984^pEPA 1982^qSame for all isomers