

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of heptachlor and heptachlor epoxide is located in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of heptachlor and heptachlor epoxide is located in Table 4-2.

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Table 4-1. Chemical Identity of Heptachlor and Heptachlor Epoxide^a

| Characteristic | Heptachlor | Heptachlor epoxide |
|--------------------------|---|--|
| Synonym(s) | 3-Chlorochlordene; 1,4,5,6,7,8,8a-hepta- chloro-3a,4,7,7a-tetrahydro- 4,7-methanoindene; 1,4,5,6,7,8,8-heptachloro- 3A,4,5,5a tetrahydro; alpha- dicyclopentadiene, 3,4,5,6,8,8a heptachloro, and others | Epoxyheptachlor; 1,4,5,6,7,8,8a-hepta- chloro-2,3-epoxy-3a,4,7,7a-tetra- hydro-4,7-methanoindene; 4,7-methanoindan, 1,4,5,6,7,8, 8-heptachloro-2,3-epoxy- 3a,4,7,7a-tetrahydro-; 2,5-methano-2h-indeno (1,2-b)oxirene, 2,3,4,5,6,7, 7-heptachloro-1a,1b, 5,5a,6,6a-hexahydro-, (1aalpha,1bbeta,2alpha,5alpha, 5abeta,6beta,6aalpha)- |
| Registered trade name(s) | Basaklor; Gold Crest H-60; Termide; Heptagran; Heptagranox; Heptamak; Heptamul; Soleptax; Velsicol 104 | Velsicol 53-CS-17 |
| Chemical formula | C ₁₀ H ₅ Cl ₇ | C ₁₀ H ₅ Cl ₇ O |
| Chemical structure | | |
| Identification numbers: | | |
| CAS registry | 76-44-8 | 1024-57-3 |
| NIOSH RTECS | PC0700000 | |
| EPA hazardous waste | P059 | D031 |
| OHM/TADS | 7216526 | 833300216 |
| DOT/UN/NA/IMDG shipping | UN 2761, UN2782, UN 2995, UN2996, IMO 3.0, IMO 6.1 | UN 2761, UN2782, UN 2995, UN2996, IMO 3.0, IMO 6.1 |
| HSDB | 554 | 6182 |
| NCI | C00180 | |

^aAll information obtained from HSDB 2007a for heptachlor or HSDB 2007b for heptachlor epoxide unless otherwise noted.

CAS = Chemical Abstracts Services; DOT/UN/NA/IMDG = 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 Heptachlor and Heptachlor Epoxide^a

| Property | Heptachlor | Heptachlor epoxide |
|--------------------------|--|--|
| Molecular weight | 373.32 | 389.40 |
| Color | White (pure); tan (technical grade) ^b | White ^b |
| Physical state | Crystalline solid | Crystalline solid ^b |
| Melting point | 95–96 °C (pure); 46–74 °C (technical grade) ^c | 160–161.5 °C |
| Boiling point | 145 °C | No data |
| Specific Gravity: | | |
| at 9 °C | 1.57 | No data |
| Odor | Camphor-like | No data |
| Odor threshold: | | |
| Water | No data | No data |
| Air | 0.3 mg/m ³ | 0.3 mg/m ³ |
| Solubility: | | |
| Water at 25 °C | 0.05 mg/L ^d | 0.275 mg/L ^d |
| Organic solvent(s) | Soluble in most organic solvents | Soluble in most organic solvents ^b |
| Partition coefficients: | | |
| Log K _{ow} | 6.10 | 5.40 |
| Log K _{oc} | 4.34 ^e | 3.34–4.37 ^f |
| Vapor pressure | | |
| | 3x10 ⁻⁴ mmHg ^g at 20 °C | 1.95x10 ⁻⁵ mmHg at 30 °C ^h |
| | 3x10 ⁻⁴ mmHg at 25 °C | No data |
| Henry's law constant: | | |
| at 25 °C | 2.94x10 ⁻⁴ atm-m ³ /mol | 3.2x10 ⁻⁵ atm-m ³ /mol |
| Autoignition temperature | No data | No data |
| Flashpoint | No data | No data |
| Flammability limits | Highly flammable | Non-combustible |
| Conversion factors | 1 ppm=15.27 mg/m ³ at 25 °C, 1 atm | 1 ppm=15.93 mg/m ³ at 25 °C, 1 atm |
| Explosive limits | Non-combustible | Containers may explode when heated |

^aAll information obtained from HSDB 2007a for heptachlor or HSDB 2007b for heptachlor epoxide unless otherwise noted

^bIARC 1974

^cWorthing and Walker 1987

^dEPA 1987

^eChapman 1989

^fEstimated from Lyman et al. 1982

^gACGIH 1986

^hNash 1983