CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of mirex and chlordecone is located in Table 4-1.

	Information		
Characteristic	Mirex	Chlordecone	
Chemical name	1,1a,2,2,3,3a,4,5,5,5a,5b,6-Dodeca- chlorooctahydro-1,3,4-metheno- 1H-cyclobuta[cd]- pentalene	1,1a,3,3a,4,5,5,5a,5b,6-Deca- chlorooctahydro-1,3,4- metheno- 2H-cyclobuta[cd] pentalen-2-one	
Synonym(s) and registered trade name(s)	1,2,3,4,5,5-Hexachloro- 1,3-cyclopentadiene dimer ^b ; dodecachlorooctahydro- 1,3,4-metheno-1H-cyclobuta[cd] pentalene ^b	Decachloroketone ^c ; decachloro- octahydro-1,3,4-metheno- 2H-cyclobuta[cd]pentalen-2-one ^c GC 1189; Kepone; Merex ^c	
	CG-1283; Dechlorane; ENT 25719 ^d		
Chemical formula	C10Cl12	C ₁₀ Cl ₁₀ O	
Chemical structure			
CAS Registry Number	2385-85-5	143-50-0	

Table 4-1. Chemical Identity of Mirex and Chlordecone^a

^aAll information obtained from Budavari et al. 1989, except where noted. ^bIARC 1979. ^cIARC 1979. ^dNLM 2020.

CAS = Chemical Abstracts Service

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of mirex and chlordecone is located in

Table 4-2.

Table 4-2. Physical and Chemical Properties of Mirex and Chlordecone

	Information	
Property	Mirex	Chlordecone
Molecular weight	545.59	490.68
Color	Snow-white	Tan-white ^b
Physical state	Crystalline solid	Crystalline solid
Melting point	485°C (decomposes)	350°C (decomposes) ^b
Boiling point	No data	No data
Density at 25°C	No data	No data
Odor	Odorless	Odorless ^c
Odor threshold	5.0667 mg/m ^{3 d}	
Solubility:		
Water	Practically insoluble 0.60 mg/L ^e insoluble ^f 0.2 mg/L at 24°C (practical grade) ^f	Slightly soluble 3.0 mg/L ^e practically insoluble ^b
Organic solvents	Dioxane (15.3%); xylene (14.3%); benzene (12.2%); CCl ₄ (7.2%); methyl ethyl ketone (5.6%)	Soluble in hydrocarbon solvents, alcohols, ketones
Partition coefficients:		
Log Kow	5.28 ^g	4.50 ^h
Log K _{oc}	3.763 ^f	3.38–3.415 ^h
Vapor pressure at 25°C	3x10 ⁻⁷ mm Hg ^f	<3x10⁻ ⁷ mm Hg⁵
Henry's law constant:		
at 20°C	839.37 Pa m ³ /mole ⁱ	2.50x10 ⁻⁸ atm
At 22°C	5.16x10 ⁻⁴ atm m ³ /mole ^j	m ³ /mole ^h
Autoignition temperature	Nonflammable ^b	Nonflammable
Flashpoint	No data	No data
Flammability limits	Nonflammable ^d Supports combustion	Nonflammable
Conversion factors	1 ppm=0.041 mg/m ³	1 ppm=0.046 mg/m ³
Explosive limits	No data	No data

^aAll information obtained from Budavari et al. 1989, except where noted.
^bIARC 1979.
^cVerschueren 1983.
^dNLM 2020.
^eKenaga 1980.
^fIARC 1979.
^gNiimi 1991.
^hHoward 1991.
ⁱDomine et al. 1992.
ⁱYin and Hassett 1986.

CCl₄ = carbon tetrachloride