

## 4. CHEMICAL AND PHYSICAL INFORMATION

### 4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of toxaphene is located in Table 4-1.

### 4.2 PHYSICAL AND CHEMICAL PROPERTIES

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

Toxaphene is not a single molecular substance; rather, it is a complex mixture of congeners including chlorinated bornanes, bornenes, bornadienes, camphenes, and dihydrocamphenes (de Geus et al. 1999).

The congeners typically contain 6–10 chlorine atoms each (de Geus et al. 1999; Lau et al. 1996).

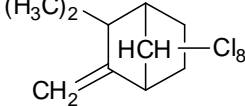
Representative structures for the different types of toxaphene congeners are shown in Figure 4-1.

Although thousands of toxaphene congeners are theoretically possible based on these structures, only a few hundred are expected to be present at significant concentrations in technical toxaphene (de Geus et al. 1999; Lamb et al. 2008; Simon and Manning 2006).

The chemical structure of specific toxaphene congeners has been described using a variety of nomenclature systems, some of which are summarized in de Geus et al. (1999). This Toxicological Profile for Toxaphene employs the nomenclature system developed by Dr. Harun Parlár to refer to specific congeners (Coelhan and Parlár 1996).

## 4. CHEMICAL AND PHYSICAL INFORMATION

**Table 4-1. Chemical Identity of Toxaphene**

Characteristic	Information	Reference
Chemical name	Toxaphene	ChemIDplus Advanced 2010
Synonym(s)	Campheclor; chlorinated camphene; polychlorocamphene; chlorocamphene; octachlorocamphene; technical toxaphene	ChemIDplus Advanced 2010
Registered trade name(s)	Agricide Maggot Killer; Alltox; Camphofene Huilex; Geniphene; Hercules 3956; Hercules Toxaphene; Motox; Penphene; Phenicide; Phenatox; Strobane-T; Synthetic 3956; Toxakil	IARC 1979
Chemical formula	C <sub>10</sub> H <sub>10</sub> Cl <sub>8</sub> (approximately)	O'Neil et al. 2006
Chemical structure <sup>a</sup>		Paris and Lewis 1973
Identification numbers:		
CAS Registry	8001-35-2	ChemIDplus Advanced 2010; NIOSH 2005
NIOSH RTECS	XW5250000	
EPA Hazardous Waste	P123	HSDB 2010
DOT/UN/NA/IMCO	NA 2761/toxaphene	NIOSH 2005
HSDB	1616	HSDB 2010

<sup>a</sup>Structure representative of the predominant chlorinated camphene compounds present in technical toxaphene.

CAS = Chemical Abstracts Services; 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; IARC = International Agency for Research on Cancer; NIOSH = National Institute for Occupational Safety and Health; RTECS = Registry of Toxic Effects of Chemical Substances

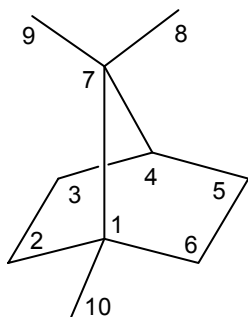
## 4. CHEMICAL AND PHYSICAL INFORMATION

**Table 4-2. Physical and Chemical Properties of Toxaphene<sup>a</sup>**

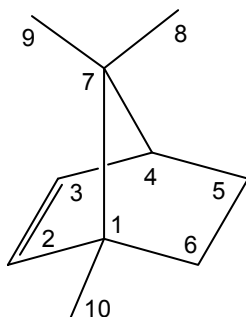
Property	Information	Reference
Molecular weight	431.8 (approximately)	BCPC 2003
Color/form	Yellow, waxy, amber	NIOSH 2005; O'Neil et al. 2006
Physical state	Solid	O'Neil et al. 2006
Melting point	65–90°C	O'Neil et al. 2006
Boiling point	Not applicable (dechlorinates at 155°C)	O'Neil et al. 2006
Density at 25°C	1.65 g/cm <sup>3</sup>	BCPC 2003
Odor	Mild, piney, chlorine- and camphor-like odor	NIOSH 2005
Odor threshold:		
Air	0.14 ppm (detection)	Sigworth 1965; Ruth 1986
Water	2.4 mg/m <sup>3</sup> 0.14 ppm (detection)	HSDB 2010
Solubility:		Murphy et al. 1987
Water	0.55 mg/L	
Organic solvent(s)	Freely soluble in aromatic hydrocarbons Readily soluble in organic solvents, including petroleum oils	BCPC 2003; O'Neil et al. 2006
Partition coefficients:		
Log K <sub>ow</sub>	3.3–6.64	EPA 1981; Fisk et al. 1999
Log K <sub>oc</sub>	3–5	EPA 1981; Soubaneh et al. 2008; Wauchope et al. 1992
Vapor pressure	6.69x10 <sup>-6</sup> mm Hg at 20°C	Murphy et al. 1987
Henry's law constant	6x10 <sup>-6</sup> atm·m <sup>3</sup> /mol at 20°C	Murphy et al. 1987
Autoignition temperature	No data	
Flashpoint	135°C (closed cup, 60% solution) 115°C (tag closed cup, 90% solution)	HSDB 2010
Flammability limits in air	Solid is not flammable, but is usually dissolved in combustible liquid	HSDB 2010
Conversion factors (25°C)	1 ppm x 17.95(average)=1 mg/m <sup>3</sup> ; 1 mg/m <sup>3</sup> x 0.056 (average)=1 ppm	Calculated
Explosive limits	No data	

<sup>a</sup>Technical toxaphene is a complex mixture of hundreds of polychlorinated bicyclic terpenes consisting predominantly of chlorinated camphenes (Jansson and Wideqvist 1983; Paris and Lewis 1973). Toxaphene contains 67–69% chlorine by weight (de Geus et al. 1983).

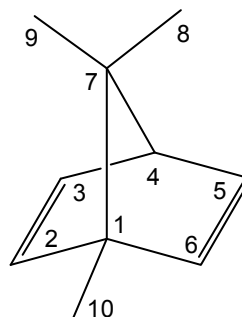
## 4. CHEMICAL AND PHYSICAL INFORMATION

**Figure 4-1. Representative Carbon Skeleton Structures of the Toxaphene Congeners with Numbered Carbon Atoms<sup>a</sup>**

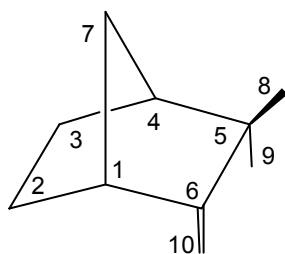
Bornane



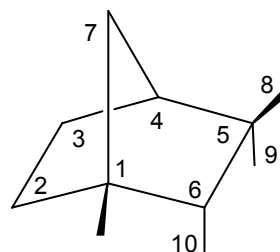
Bornene



Bornadiene



Camphene



Dihydrocamphene

<sup>a</sup>Congeners typically contain 6–10 chlorine atoms.

Source: de Geus et al. 1999