METHOXYCHLOR 139

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

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

Methoxychlor is produced commercially in the United States as a technical grade containing 88–90% of the pure chemical and 10-12% of impurities consisting of isomers and other reaction products (IARC 1979; Lamoureux and Feil 1980). Twenty-five of these impurities were characterized in studies conducted on technical methoxychlor; evidence for >50 impurities was obtained through gas chromatography/mass spectrometry (GC/MS) (Lamoureux and Feil 1980). Purification of technical grade (nominally 90%) 1,1,1-trichloro-2,2-bis(4-methoxyphenyl)ethane (p,p'-methoxychlor; p,p'-DMDT) by recrystalization gave 76% p,p'-methoxychlor (99.8% pure by normal phase high performance liquid chromatography [HPLC]) and 24% impurities (West et al. 1982). The impurities were found to contain approximately 40 components. The major components were identified (HPLC and GC/MS) using reference standards. Component identities and percent (w/w) in technical grade methoxychlor were found to be as follows: 1,1,1,2-tetrachloro-2-(4-methoxyphenyl)ethane (1.73%), 1,1,1-trichloro-2-(2-methoxyphenyl)ethane phenyl)-2-(4-methoxyphenyl)ethane (o,p'-methoxychlor; o,p'-DMDT; 4.03%), 1,1-dichloro-2,2-di(4-methoxyphenyl)ethene (DMDE; 0.39%), a condensation product of p,p'-methoxychlor (p, p')-DMDT; 0.48%), a condensation product of (p, p')-methoxychlor (p, p')-DMDT; 0.4%), and 1,2,2,2-tetrakis(4-methoxybenzyl)ethene (0.5%). The percentages were calculated relative to the quantity of methoxychlor contained in technical grade material and were found to vary depending upon manufacturing conditions. Another impurity is 1-chloro-1,2,2-tris(4-methoxyphenyl)ethene (chlorotrianisene; TACE), a triphenylethylene derivative, that exhibits estrogenic/anti-estrogenic characteristics. Other impurities include polycylic hydrocarbons (e.g., 3,6-dimethoxy-9,10-bis (p-methoxyphenyl)phenanthrene, tetrakis(p-methoxyphenyl)ethylene, and 3,6,11,14-tetramethoxydibenzo(g,p)chrysene), which have been studied for mutagenicity and putative carcinogenicity (Grant et al. 1976). The substance, 3,6,11,14-tetramethoxydibenzo(g,p)chrysene, was found to be mutagenic.

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-1. Chemical Identity of Methoxychlor

| Characteristic | Information | Reference |
|---|---|--|
| Chemical name | Methoxychlor | Howard 1991 |
| Synonym(s) | 2,2-bis(p-methoxyphenyl)- 1,1,1-trichoroethane; 1,1,1-trichloro-2,2- bis(4-methoxyphenyl) ethane; methoxy-DDT; 1,1r-(2,2,2- trichloroethylidene)-bis(4- methoxybenzene) | HSDB 2000 |
| Registered trade name(s) | Marlate® Metox® Prentox®; Methoxcide® | EPA 1988b; HSDB 2000; Sittig 1980 |
| Chemical formula | $C_{16}H_{15}CI_3O_2$ | Howard 1991 |
| Chemical structure | | EPA 1988c |
| | CH ₃ O OCH ₃ | |
| | 1,1,1-Trichloro-2,2-bis(4-meth oxyphenyl)ethane (<i>p,p</i> '-methoxy chlor; DMDT) | |
| Identification numbers: CAS registry NIOSH RTECS EPA hazardous waste OHM/TADS DOT/UN/NA/IMCO shipping | 72-43-5 KJ 3675000 U247; D014 OHM 7216536 DOT 2761 UN 2761 NA 2761 IMCO 6.1 | Howard 1991 Sax and Lewis 1989 HSDB 2000 HSDB 2000 Sax and Lewis 1989 HSDB 2000 |
| HSDB NCI | 1173 C00497 | HSDB 2000 HSDB 2000 |

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; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substance

4.2 PHYSICAL AND CHEMICAL PROPERTIES

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

Table 4-2. Physical and Chemical Properties of Methoxychlor

| Property | Information | Reference |
|--|---|--|
| Molecular weight | 345.65 | Howard 1991 |
| Color | Pale yellow | EPA 1988c |
| Physical state | Crystalline solid | EPA 1988c |
| Melting point | 89 EC | HSDB 2000 |
| | 77 EC (technical grade) No data (decomposes) | Montgomery and Welkom 1990 |
| Density: at 25 EC | 1.41 g/cm ³ | Montgomery and Welkom 1990 |
| Odor | Slightly fruity; musty; chlorine-like | HSDB 2000; Sigworth 1965 |
| Odor threshold: Water 60 EC Air | 4.7 ppm No data | Sigworth 1965 |
| Solubility: Water at 25 EC at 15 EC at 24 EC at 35 EC at 45 EC | 0.045 mg/L 0.02 mg/L 0.04 mg/L 0.095 mg/L 0.185 mg/L | |
| Organic solvent(s) | Soluble in chlorinated aromatic solvents, ketonic solvents, ethanol, methylene chloride, methylated naphthalene, carbon tetrachloride, chloroform, xylene, methanol, petroleum ether, benzene | Budavari et al. 1989; EPA 1988a; HSDB 2000; Montgomery and Welkom 1990 |
| Partition coefficients: Log K_{ow} Log K_{oc} | 4.68–5.08 4.9 | Howard 1991 Montgomery and Welkom 1990 |
| Vapor pressure at 25 EC | 1.4x10 ⁻⁶ mmHg (estimated) | Howard 1991 |
| Henry's law constant: at 25 EC | 1.6x10 ⁻⁵ atm-m ³ /mol (estimated) | Howard 1991 |
| Autoignition temperature | No data | |
| Flashpoint | No data | |
| Flammability limits | No data | |
| Conversion factors ^a | No data | |
| Explosive limits | No data | |

^aExists partially in particulate form in air. Conversion factors are only applicable for compounds that are entirely in the vapor phase.