

CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

When we refer to DDT, we are generally referring to *p,p'*-DDT, which was produced and used for its insecticidal properties. However, technical-grade DDT, the grade that was generally used as an insecticide, was composed of up to 14 chemical compounds, of which only 65–80% was the active ingredient, *p,p'*-DDT. The other components included 15–21% of the nearly inactive *o,p'*-DDT, up to 4% of *p,p'*-DDD, and up to 1.5% of 1-(*p*-chlorophenyl)-2,2,2-trichloroethanol (Metcalf 1995).

The chemical formulas, structures, and identification numbers for *p,p'*-DDT, *p,p'*-DDE, *p,p'*-DDD, *o,p'*-DDT, *o,p'*-DDE, and *o,p'*-DDD are listed in Table 4-1. The latter five compounds are either impurities or metabolites of technical DDT.

Table 4-1. Chemical Identity of *p,p'*- and *o,p'*-DDT, DDE, and DDD^a

Characteristic	Information		
Chemical name	<i>p,p'</i> -DDT	<i>p,p'</i> -DDE	<i>p,p'</i> -DDD
Synonym(s) and registered trade names	4,4'-DDT; 1,1,1-trichloro-2,2-bis(<i>p</i> -chlorophenyl)ethane; dichlorodiphenyltrichloroethane; DDT; 1,1'-(2,2,2-trichloroethylidene) bis(4-chlorobenzene); α-α-bis(<i>p</i> -chlorophenyl)-β,β,β-trichloroethane; Genitox; Anofex; Detoxan; Neocid; Gesarol; Pentachlorin; Dicophane; Chlorophenothane ^b	4,4'-DDE; dichlorodiphenyl-dichloroethane; 1,1-dichloro-2,2-bis(<i>p</i> -chlorophenyl)ethylene; 1,1'-(2,2-dichloroethylidene) bis(4-chlorobenzene); DDE	4,4'-DDD; dichlorodiphenyl-dichloroethane; DDD; 1,1-dichloro-2,2-bis(<i>p</i> -chlorophenyl)ethane; 1,1-bis(4-chlorophenyl)-2,2-dichloroethane; TDE; tetrachlorodiphenylethane; DDD; Rothane; Dilene; TDE
Chemical formula	C ₁₄ H ₉ Cl ₅	C ₁₄ H ₈ Cl ₄	C ₁₄ H ₁₀ Cl ₄
Chemical structure			
CAS Registry Number	50-29-3	72-55-9	72-54-8

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Table 4-1. Chemical Identity of *p,p'*- and *o,p'*-DDT, DDE, and DDD^a

Characteristic	Information		
Chemical name	<i>o,p'</i> -DDT	<i>o,p'</i> -DDE	<i>o,p'</i> -DDD
Synonym(s) and registered trade names	2,4'-DDT; 1,1,1-trichloro-2-(<i>o</i> -chlorophenyl)-2-(<i>p</i> -chlorophenyl)ethane; <i>o,p'</i> -dichlorodiphenyl-trichloroethane	2,4'-DDE; 1,1-dichloro-2-(<i>o</i> -chlorophenyl)-2-(<i>p</i> -chlorophenyl)ethylene; 1-chloro-2-(2,2-dichloro-1-(4-chlorophenyl)ethenyl)benzene	2,4'-DDD; Mitotane; <i>o,p'</i> -DDD; 1,1-dichloro-2-(<i>o</i> -chlorophenyl)-2-(<i>p</i> -chlorophenyl)ethane; <i>o,p'</i> -TDE; Choditane; 2-(<i>o</i> -chlorophenyl)-2-(<i>p</i> -chlorophenyl); Lysodren
Chemical formula	C14H9Cl5	C14H8Cl4	C14H10Cl4
Chemical structure			
CAS Registry Number	789-02-6	3424-82-6	53-19-0

^aHoward and Neal (1992) except where noted.

^bKlassen et al. 1991.

CAS = Chemical Abstracts Service

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Technical DDT is a white amorphous powder that melts over the range of 80–94°C (Metcalfe 1995).

Physical and chemical properties of *p,p'*-DDT, *p,p'*-DDE, *p,p'*-DDD, *o,p'*-DDT, *o,p'*-DDE, and *o,p'*-DDD are listed in Table 4-2.

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Table 4-2. Physical and Chemical Properties of *p,p'*- and *o,p'*-DDT, DDE, and DDD^a

Property	<i>p,p'</i> -DDT	<i>p,p'</i> -DDE	<i>p,p'</i> -DDD
Molecular weight	354.5	318.03 ^b	320.05 ^b
Color	Colorless crystals	White	Colorless crystals, white powder
Physical state	Solid	Crystalline solid	Solid
Melting point	108.5–109°C	89°C ^b	109–110°C ^b
Boiling point	Decomposes; 185–187 at 0.05 mmHg	336°C ^b	350°C ^b
Density at 20°C	1.56 g/cm ³	No data	1.385 g/cm ³
Odor	Odorless or weak aromatic odor ^c	No data	Odorless
Odor threshold:			
Water	0.35 mg/kg ^d	No data	No data
Air	No data	No data	No data
Solubility:			
Water	0.025 mg/L at 25°C ^b	0.12 mg/L at 25°C ^b	0.05 mg/L at 25°C
Organic solvents	1,000 g/L in cyclohexane and dioxane; 850 g/L in dichloromethane; 770 g/L in benzene; 600 g/L in xylene; 50 g/L in acetone; 470 g/L in carbon tetrachloride; 310 g/L in chloroform; 270 g/L in diethyl ether; 60g/L in ethanol; 40 g/L in methanol	Lipids and most organic solvents	No data
Partition coefficients:			
Log K _{ow}	6.91 ^b	6.51 ^b	6.02 ^b
Log K _{oc}	5.18 ^e	4.70 ^f	5.18 ^g
Vapor pressure at 20°C	1.60x10 ⁻⁷ , torr ^b	6.0x10 ⁻⁶ at 25°C, torr ^b	1.35x10 ⁻⁶ at 25°C, torr ^b
Henry's law constant at 25°C	8.3x10 ⁻⁶ atm-m ³ /mol ^b	2.1x10 ⁻⁵ atm-m ³ /mol ^b	4.0x10 ⁻⁶ atm-m ³ /mol ^b
Autoignition temperature	No data	No data	No data
Flashpoint	72.2–77.2 °C	No data	No data
Flammability limits	No data	No data	No data
Conversion factors			
Ppm (v/v) to mg/m ³ in air at 20°C	Not applicable ^h	Not applicable ^h	Not applicable ^h
mg/m ³ to ppm (v/v) in air at 20°C	Not applicable	Not applicable	Not applicable
Explosive limits	No data	No data	No data

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Table 4-2. Physical and Chemical Properties of *p,p'*- and *o,p'*-DDT, DDE, and DDD^a

Property	<i>o,p'</i> -DDT	<i>o,p'</i> -DDE	<i>o,p'</i> -DDD
Molecular weight	354.49 ^b	318.03 ^b	320.05 ^b
Color	White crystalline powder ^d	No data	No data
Physical state	Solid	No data	Solid
Melting point	74.2°C ^c	No data	76–78°C
Boiling point	No data	No data	No data
Density at 20°C	0.98–0.99 g/cm ³	No data	No data
Odor	Odorless or weak aromatic odor ^c	No data	No data
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Solubility:			
Water	0.085 mg/L at 25°C ^b	0.14 mg/L at 25°C	0.1 mg/L at 25°C ^b
Organic solvents	No data ⁱ	No data ⁱ	Soluble in ethanol, isoctane, carbon tetrachloride ^h
Partition coefficients:			
Log K _{ow}	6.79 ^e	6.00 ^b	5.87 ^b
Log K _{oc}	5.35 ^g	5.19 ^g	5.19 ^g
Vapor pressure at 20°C	1.1x10 ⁻⁷ , torr ^b	6.2x10 ⁻⁶ at 25°C, torr ^b	1.94x10 ⁻⁶ at 30°C, torr ^b
Henry's law constant at 25°C	5.9x10 ⁻⁷ atm-m ³ /mol ^b	1.8x10 ⁻⁵ atm-m ³ /mol ^b	8.17x10 ⁻⁶ atm-m ³ /mol ^b
Autoignition temperature	No data	No data	No data
Flashpoint	No data	No data	No data
Flammability limits	No data	No data	No data
Conversion factors			
ppm (v/v) to mg/m ³ in air at 20°C	Not applicable ^h	Not applicable ^h	Not applicable ^h
mg/m ³ to ppm (v/v) in air at 20°C	Not applicable	Not applicable	Not applicable
Explosive limits	No data	No data	No data

^aMacbean 2011, unless otherwise noted.^bHoward and Meylan 1997.^cSax 1979.^dVerschueren 1983.^eSwann et al. 1981.^fSabljic 1984.^gMeylan et al. 1992 (values estimated from a fragment constant method).^hExists partially in particulate form in air. Conversion factors are only applicable for compounds that are entirely in the vapor phase.