



Uploaded to the VFC Website

▶▶▶ 2021 ◀◀◀

This Document has been provided to you courtesy of Veterans-For-Change!

Feel free to pass to any veteran who might be able to use this information!

For thousands more files like this and hundreds of links to useful information, and hundreds of "Frequently Asked Questions, please go to:

[Veterans-For-Change](#)

If Veterans don't help Veterans, who will?

Note:

VFC is not liable for source information in this document, it is merely provided as a courtesy to our members & subscribers.



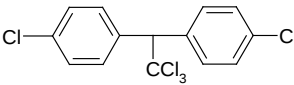
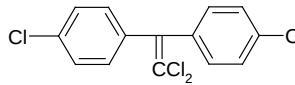
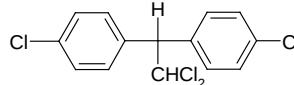
CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

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).

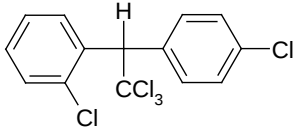
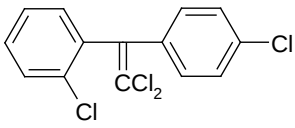
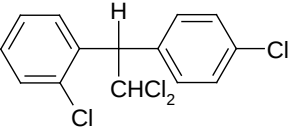
The chemical formulas, structures, and identification numbers for *p,p'*-DDT, *p,p'*-DDE, *p,p'*-DDD, *o,p'*-DDT, *o,p'*-DDE, and *o,p'*-DDD are listed in Table 4-1. The latter five compounds are either impurities or metabolites of technical DDT.

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; dichlorodiphenyl trichloroethane; 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; 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

4. CHEMICAL AND PHYSICAL INFORMATION

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	C ₁₄ H ₉ Cl ₅	C ₁₄ H ₈ Cl ₄	C ₁₄ H ₁₀ Cl ₄
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 (Metcalf 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.

4. CHEMICAL AND PHYSICAL INFORMATION

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

4. CHEMICAL AND PHYSICAL INFORMATION

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 ^j	No data ^j	Soluble in ethanol, isooctane, 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.^fSabljić 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.