

CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

2,4-D is a free acid, phenoxy herbicide belonging to the phenoxyacetic acid chemical family, which is widely used in the United States. While the free acid is itself used as an herbicide, there are nine forms of 2,4-D registered as active ingredients in end use products. These include salts, amines, and esters of 2,4-D (EPA 2005a). Derivatives include the sodium salt, diethanolamine salt, dimethyl amine salt, isopropylamine salt, triisopropanolamine salt, butoxyethyl ester, ethylhexyl ester, and isopropyl ester. Almost 90–95% of total 2,4-D global use is accounted for by the dimethyl amine salt and ethylhexyl ester (Charles et al. 2001).

Formulations of 2,4-D and its derivatives vary in their chemical properties and behavior in the environment. However, most quantified analyses of 2,4-D and its derivatives are expressed in terms of the free acid (EPA 2005a).

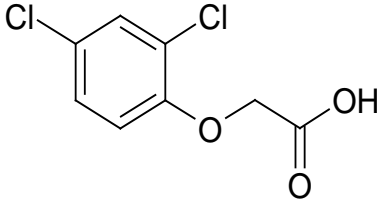
Information regarding the chemical identity of 2,4-D and its derivatives are provided in Tables 4-1 and 4-2, respectively.

Table 4-1. Chemical Identity of 2,4-D^a

Characteristic	Information
Chemical name	2,4-Dichlorophenoxyacetic acid
Synonym(s)	2,4-D; 2,4-D Acid; Acetic acid, (2,4-dichlorophenoxy)-
Registered trade name(s) ^b	Aqua-Kleen; Citrus Fix; Pyresta; Cimarron; Restore; Rush 24; 240; AMINO; Amoxone; Chloroxone; Crop Rider; Dinoxol; Dormone; Emulsamine; Fernimine; Fernoxone; Gesapax-H; Rilof-H; Target; Arena; Campeon; Fenix; Fenix Gold; Stockton; Talion; Turuna; Valsamba; Valsamin; Barrage; Brush-Rhap; Double Up; EndRun; HardBall; Opti-Amine; Trump-Card; Unison; Broadrange; Foundation; Weco Max; Brash; Phenoxy 088; Rugged; Strike; Charge; Dacomin; Chaser; Clean amine; Colt; Crossbow; Rifle; Saber; Salvo; Savage; Shotgun; Whiteout; Defy; Dical; Harvade; Willomine; Duplosan; Dyvel; Lotus; Topshot; U 46; Weedmaster; Speed-Mix; Gen-Amin; Gen-Ester; Grotex Complex; Grox; Trago

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Table 4-1. Chemical Identity of 2,4-D^a

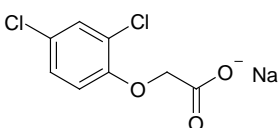
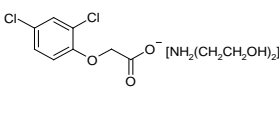
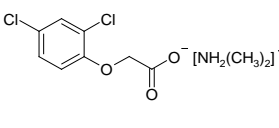
Characteristic	Information
Chemical formula	C ₈ H ₆ Cl ₂ O ₃
Chemical structure	
CAS Registry Number	94-75-7

^aAll information obtained from HSDB (2015), unless otherwise noted.

^bMeister et al. 2014.

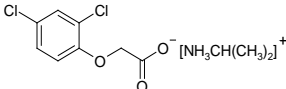
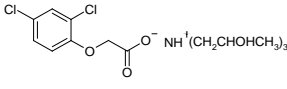
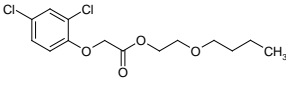
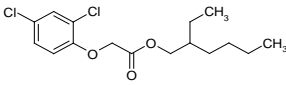
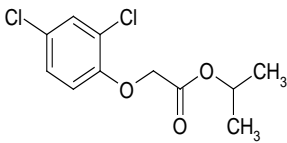
2,4-D = 2,4-dichlorophenoxyacetic acid; CAS = Chemical Abstracts Services; HSDB = Hazardous Substance Data Bank

Table 4-2. Chemical Identity of 2,4-D Derivatives

Characteristic	Information ^a		
Chemical name	2,4-D Sodium ^b	2,4-D Diethanolamine ^c	2,4-D Dimethylamine
Synonym(s)	Acetic acid, (2,4-dichlorophenoxy)-, sodium salt; Sodium 2,4-dichlorophenoxyacetate; 2,4-Dichlorophenoxyacetic acid, sodium salt; 2,4-D Na ^b	2,4-Diolamine; Acetic acid, (2,4-dichlorophenoxy)-, diethanolamine salt; 2,4-D Bis(2-hydroxyethyl) ammonium; 2,4-D DEA ^{b,c}	Acetic acid, (2,4-dichlorophenoxy)-, dimethylamine (1:1); (2,4-Dichlorophenoxy)acetic acid dimethylamine salt; Dimethylammonium (2,4-dichlorophenoxy)acetate; 2,4-D DMA
Registered trade name(s)	See 2,4-D in Table 4-1	See 2,4-D in Table 4-1	See 2,4-D in Table 4-1
Chemical formula	C ₈ H ₅ Cl ₂ O ₃ .Na ^b	C ₈ H ₆ Cl ₂ O ₃ .C ₄ H ₁₁ NO ₂ ^b	C ₈ H ₆ Cl ₂ O ₃ .C ₂ H ₇ N
Chemical structure ^c			
CAS Registry Number	2702-72-9	5742-19-8	2008-39-1

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Table 4-2. Chemical Identity of 2,4-D Derivatives

Characteristic	Information ^a		
Chemical name	2,4-D Isopropylamine ^c	2,4-D Triisopropanolamine ^c	2,4-D Butoxyethyl ester
Synonym(s)	2,4-D- isopropylammonium; Acetic acid, (2,4-dichlorophenoxy)-, isopropylamine salt; 2-Propanamine, (2,4-dichlorophenoxy) acetate; 2,4-D IPA ^{b,c}	Acetic acid, (2,4-dichlorophenoxy)-, triisopropanolamine salt; 2,4-D- tris(2-hydroxypropyl) ammonium; 2-Propanol, 1,1',1''-nitritoltris-, (2,4-dichlorophenoxy) acetate; 2,4-D TIPA ^{b,c}	Acetic acid, (2,4-dichlorophenoxy)-, 2-butoxyethyl ester; 2,4-Dichlorophenoxy- acetic acid, butoxyethyl ester; 2,4-D BEE
Registered trade name(s)	See 2,4-D in Table 4-1	See 2,4-D in Table 4-1	See 2,4-D in Table 4-1
Chemical formula	C ₈ H ₆ Cl ₂ O ₃ .C ₃ H ₉ N ^b	C ₈ H ₆ Cl ₂ O ₃ .C ₉ H ₂₁ NO ₃ ^b	C ₁₄ H ₁₈ Cl ₂ O ₄
Chemical structure ^c			
CAS Registry Number	5742-17-6	32341-80-3	1929-73-3
Chemical name	2,4-D Ethylhexyl ester	2,4-D Isopropyl ester	
Synonym(s)	Isooctyl(2-ethylhexyl) 2,4-dichlorophenoxy- acetate; 2,4-D, 2-ethylhexyl; 2-Ethylhexyl (2,4-dichlorophenoxy) acetate; Acetic acid, (2,4-dichlorophenoxy)-, 2-ethylhexyl ester; 2,4-D EHE	Acetic acid, (2,4-dichlorophenoxy)-, isopropyl ester; Acetic acid, (2,4-dichlorophenoxy)-, 1-methylethyl ester; 2,4-Dichlorophenoxyacetic acid isopropyl ester; Isopropyl (2,4-dichlorophenoxy)acetate; Isopropyl 2,4-D ester; 2,4-D IPE	
Registered trade name(s)	See 2,4-D in Table 4-1	See 2,4-D in Table 4-1	
Chemical formula	C ₁₆ H ₂₂ Cl ₂ O ₃	C ₁₁ H ₁₂ Cl ₂ O ₃	
Chemical structure ^c			
CAS Registry Number	1928-43-4	94-11-1	

^aAll information obtained from HSDB (2015), unless otherwise noted.

^bMeister et al. 2014.

^cEPA 2005a.

2,4-D = 2,4-dichlorophenoxyacetic acid; CAS = Chemical Abstracts Services; EPA = Environmental Protection Agency; HSDB = Hazardous Substance Data Bank

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4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of 2,4-D and its derivatives are provided in Tables 4-3 and 4-4, respectively.

Table 4-3. Physical and Chemical Properties of 2,4-D^a

Property	Information
Molecular weight	221.03
Color	White to yellow
Physical state	Crystalline powder
Melting point	138°C
Boiling point	160°C (at 4 mm Hg)
Density/specific gravity: at 25°C	1.42
Odor	Odorless; slightly phenolic
Odor threshold	3.13 mg/kg
Solubility:	
Water at 20°C	540 mg/L
Water at 25°C	677 mg/L
Organic solvents at 20°C:	
Ethanol	1,250 g/kg
Diethyl ether	243 g/kg
Heptane	1.1 g/kg
Toluene	6.7 g/kg
Xylene	5.8 g/kg
Octanol	120 g/L (25°C)
Partition coefficients:	
Log K _{ow}	2.81
Log K _{oc}	19.6–135.7
Vapor pressure at 20°C	1.40x10 ⁻⁷ mm Hg
Henry's law constant at 20°C	9.75x10 ⁻⁸ atm-m ³ /mol
Autoignition temperature	No data
Flashpoint	Not combustible
Flammability limits	No data
Conversion factors	No data
Explosive limits	No data

^aAll information obtained from HSDB (2015).

2,4-D = 2,4-dichlorophenoxyacetic acid

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Table 4-4. Physical and Chemical Properties of 2,4-D Derivatives^a

Property	2,4-D Sodium	2,4-D Diethanolamine
Molecular weight	243.03 ^b	326.18 ^b
Color	White ^b	Cream ^b
Physical state	Powder ^b	Powder ^b
Melting point	200°C ^c	83°C ^c
Boiling point	No data	No data
Density: at 25°C	42.2 pounds/feet ³ (0.676 g/cm ³) (bulk) ^c	0.762 g/cm ³ (bulk) ^c
Odor	No data	No data
Odor threshold:		
Water	No data	No data
Air	No data	No data
Solubility:		
Water at 25°C	4.5x10 ⁴ mg/L (unbuffered solution) ^b	8.06x10 ⁵ mg/L (unbuffered solution) ^b
Organic solvents	No data	No data
Partition coefficients:		
Log K _{ow}	Not applicable ^{b,d}	0.0224–1.65 ^b
Log K _{oc}	No data	No data
Vapor pressure at 25°C	Not applicable ^{b,d}	9.98x10 ⁻⁸ mm Hg ^b
Henry's law constant at 25°C	No data	No data
Autoignition temperature	No data	No data
Flashpoint	No data	No data
Flammability limits	No data	No data
Conversion factors	No data	No data
Explosive limits	No data	No data

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Table 4-4. Physical and Chemical Properties of 2,4-D Derivatives^a

Property	2,4-D Dimethylamine	2,4-D Isopropylamine
Molecular weight	266.1	280.04 ^b
Color	White (pure); amber (technical) ^b	Amber ^b
Physical state	Crystals (pure); aqueous liquid (technical) ^b	Aqueous liquid ^b
Melting point	85–87°C	121°C ^c
Boiling point	Decomposition	No data
Density/specific gravity: at 20°C	1.23 ^c	1.15 ^c
Odor	Odorless	No data
Odor threshold:		
Water	No data	No data
Air	No data	No data
Solubility:		
Water at 25°C	3.0x10 ⁶ g/mL (20°C)	1.74x10 ⁵ g/mL (pH 5) 4.36x10 ⁵ g/mL (pH 7) 3.31x10 ⁵ g/mL (pH 9) (unbuffered solutions) ^b
Organic solvents	Soluble in methyl, ethyl, and isopropyl alcohols, and acetone; insoluble in kerosene and diesel oil	No data
Organic solvents at 20°C		
Acetonitrile	1.06 g/100 mL	
Methanol	>50 g/100 mL	
Toluene	0.165 g/100 mL	
n-Hexane	0.00357 g/100 mL	
Octanol	5.41 g/100 mL	
Partition coefficients:		
Log K _{ow}	0.65	Not applicable ^{b,d}
Log K _{oc}	1.85–2.13	No data
Vapor pressure at 25°C	1 x10 ⁻⁷ mm Hg ^b	Not applicable ^{b,d}
Henry's law constant at 25°C	1.4x10 ⁻¹⁶ atm-m ³ /mol ^b	No data
Autoignition temperature	No data	No data
Flashpoint	No data	No data
Flammability limits	Not flammable	No data
Conversion factors	No data	No data
Explosive limits	No data	No data

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Table 4-4. Physical and Chemical Properties of 2,4-D Derivatives^a

Property	2,4-D Triisopropanolamine	2,4-D Butoxyethyl ester
Molecular weight	412.31 ^b	321.2
Color	Amber ^b	Amber; colorless
Physical state	Aqueous liquid ^b	Liquid
Melting point	87–110°C ^c	<25°C
Boiling point	No data	89°C ^c
Density/specific gravity: at 20°C	1.21	1.232 g/cm ³
Odor	No data	Odorless (pure); fuel oil-like (technical)
Odor threshold:		
Water	No data	No data
Air	No data	No data
Solubility:		
Water at 25°C	4.61x10 ⁵ g/mL (pH 5) 4.61x10 ⁵ g/mL (pH 7) 1.04x10 ⁵ g/mL (pH 9) (unbuffered solutions) ^b	12 mg/L
Organic solvents	No data	Miscible in acetone, acetonitrile, n-hexane, and methanol; soluble in oils
Partition coefficients:		
Log K _{ow}	Not applicable ^{b,d}	4.1 ^b
Log K _{oc}	No data	No data
Vapor pressure at 25°C	Not applicable ^{b,d}	4.5x10 ⁻⁶ mm Hg
Henry's law constant at 25°C	No data	No data
Autoignition temperature	No data	No data
Flashpoint	No data	>79°C (open cup)
Flammability limits	No data	No data
Conversion factors	No data	No data
Explosive limits	No data	No data

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Table 4-4. Physical and Chemical Properties of 2,4-D Derivatives^a

Property	2,4-D Ethylhexyl ester	2,4-D Isopropyl ester
Molecular weight	333.28	263.12
Color	Golden yellow	Colorless
Physical state	Liquid	Liquid
Melting point	<-37°C	5–25°C
Boiling point	>300°C (decomposition)	240°C ^c
Density:		
at 20°C	1.148	No data
at 25°C/25°C	No data	1.255–1.270
Odor	Sweet, slightly pungent	Fuel oil-like (technical)
Odor threshold:		
Water	No data	No data
Air	No data	No data
Solubility:		
Water at 25°C	0.086 mg/L	37.3 mg/L
Organic solvents	No data	Soluble in alcohols and most oils
Partition coefficients:		
Log K _{ow}	5.78	253.8 ^c
Log K _{oc}	No data	2.78 ^b
Vapor pressure at 25°C	3.6x10 ⁻⁶ mm Hg ^b	2.32x10 ⁻⁴ mm Hg
Henry's law constant at 25°C	1.8x10 ⁻⁵ atm-m ³ /mol	2.2x10 ⁻⁶ atm-m ³ /mol ^b
Autoignition temperature	No data	No data
Flashpoint	171°C (open cup)	>79°C (open cup)
Flammability limits	No data	No data
Conversion factors	No data	No data
Explosive limits	No data	No data

^aAll information obtained from HSDB (2015), unless otherwise noted.

^bNPIC 2008.

^cEPA 2005a.

^dThe salt dissociates to acid in water; therefore, this endpoint does not apply.

2,4-D = 2,4-dichlorophenoxyacetic acid