

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Information regarding the chemical identity of dinitrophenol is located in Table 3-1.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of dinitrophenol is located in Table 3-2.

Potential metabolites of dinitrophenols in humans are listed in Table 3-3.

Table 3-1. Chemical Identity of Isomers of Dinitrophenols ^a

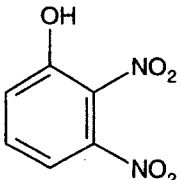
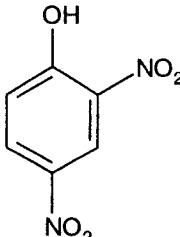
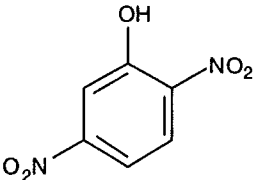
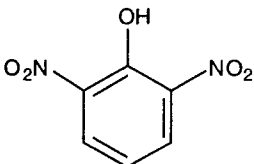
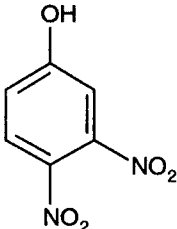
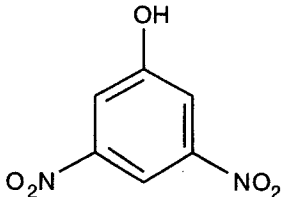
Characteristic	2,3-Dinitrophenol	2,4-Dinitrophenol	2,5-Dinitrophenol	2,6-Dinitrophenol
Synonym(s)	No data	1-Hydroxy-2,4-dinitrobenzene; α -Dinitrophenol; 2,4-DNP	γ -Dinitrophenol; 2,5-DNP ^b	β -Dinitrophenol ^b ; 2,6-DNP
Registered trade name(s)	No data	Caswell No. 392; Sulfo Black B; Sulfo Black 2B Supra; Nitro Kleanup and others	No data	No data
Chemical formula	C ₆ H ₄ N ₂ O ₅	C ₆ H ₄ N ₂ O ₅	C ₆ H ₄ N ₂ O ₅	C ₆ H ₄ N ₂ O ₅
Chemical structure				
Identification numbers:				
CAS registry ^d	66-56-8	51-28-5	329-71-5	573-56-8
NIOSH RTECS ^d	SL2700000	SL2800000	SL2900000	SL2975000
EPA hazardous waste	No data	P048	No data	No data
OHM/TADS ^{d,c}	No data	7216692	840031	7800119
DOT/UN/NA/IMCO shipping	No data	IMO 1.1 ^e ; IMO 6.1; IMO 4.1 UN 1599; UN 1320; UN 0076	IMO 1.1 ^e ; IMO 6.1; IMO 4.1 UN 1599; UN 1320; UN 0076	MO 1.1 ^e ; IMO 6.1; IMO 4.1 UN 1599; UN 1320; UN 0076
HSDB	6294	529	6304	6306
NCI	No data	No data	No data	No data

TABLE 3-1. Chemical Identity of Isomers of Dinitrophenols^a (continued)

Characteristic	3,4-Dinitrophenol	3,5-Dinitrophenol	Dinitrophenol mixture
Synonym(s)	Δ -Dinitrophenol ^d 4,5-Dinitrophenol ^d	e-Dinitrophenol ^d	Dinitrophenol solution ^d
Registered trade name(s)	No data	No data	No data
Chemical formula	C ₆ H ₄ N ₂ O ₅	C ₆ H ₄ N ₂ O ₅	(C ₆ H ₄ N ₂ O ₅)
Chemical structure			Usually a mixture of 2,3-, 2,4-, and 2,6- isomers
Identification numbers:			
CAS registry ^d	577-71-9	586-11-8	25550-58-7
NIOSH RTECS ^d	SL3000000	SL3050000	SL2625000
EPA hazardous waste	No data	No data	No data
OHM/TADS ^{d,c}	No data	No data	No data
DOT/UN/NA/IMCO shipping	No data	No data	IMO 1.1 ^e ; IMO 6.1; IMO 4.1 UN 1599; UN 1320; UN 0076
HSDB	No data	No data	6294
NCI	No data	No data	No data

^aAll information obtained from CHEMID 1995 and HSDB 1994 except where noted

^bRTECS 1992
^cOHM/TADS 1992, 1993

^dSANSS 1992
^eSax and Lewis 1987

CAS = Chemical Abstracts Service; DOT/UN/NA/IMCO = Dept. 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 and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

Table 3-2. Physical and Chemical Properties of Dinitrophenols

Characteristics	2,3-Dinitrophenol	2,4-Dinitrophenol	2,5-Dinitrophenol	2,6-Dinitrophenol
Molecular weight	184.1	184.1 ^a	184.1 ^a	184.1 ^a
Color	Yellow ^b	Yellow ^a	Yellow ^a	Light yellow ^a
Physical state	Solid ^b	Solid ^a	Solid ^a	Solid ^a
Melting point	144 °C ^c	112–114 °C ^a	108 °C ^a	63–64 °C ^a
Boiling point	No data	Sublimes ^a	No data	No data
Density (g/cm ³)	1.681 ^c	1.683 ^a	No data	No data
Odor	No data	No data	No data	No data
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Dissociation constant (pK _a)	4.89 ^b	4.09 ^d	5.22 ^d	3.71 ^d
Solubility:				
Water at 18 °C	No data	5,600 mg/L ^e	385 mg/L at 20 °C ^f	No data
Water at 35–36 °C	2,200 mg/L ^b	790 mg/L ^b	680 mg/L ^b	420 mg/L ^b
Organic solvents	No data	Solubility at 15 °C (g/100 g solution): 15.55 in ethyl acetate; 35.90 in acetone; 5.39 in chloroform; 20.05 in pyridine; 0.423 in carbon tetrachloride; 6.36 in toluene; soluble in alcohol and benzene ^a	Slightly soluble in cold alcohol; soluble in hot alcohol, ether, and fixed alkali hydroxides ^a	Slightly soluble in cold alcohol; freely soluble in chloroform, ether, boiling alcohol, and fixed alkali hydroxides ^a
Partition coefficients:				
Log K _{ow}	No data	1.54 ^g	1.75 ^g	1.37 ^g
Log K _{oc}	No data	1.69 ^{h,e}	No data	No data
Vapor pressure at 18 °C	No data	1.49x10 ⁻⁵ mm Hg ^e at 18 °C	1.05x10 ⁻³ mm Hg ^f at 20 °C	No data
Henry's law constant at 20 °C	No data	2.82x10 ⁻⁷ atm·m ³ /mol ^{f,h}	6.61x10 ⁻⁷ atm·m ³ /mol ^{f,h}	No data
Autoignition temperature	No data	No data	No data	No data
Flashpoint	No data	No data	No data	No data
Flammability limits	No data	No data	No data	No data
Conversion factors at 20 °C	1 ppm = 7.65 mg/m ³ ⁱ 1 mg/m ³ = 0.13 ppm	1 ppm = 7.65 mg/m ³ ⁱ 1 mg/m ³ = 0.13 ppm	1 ppm = 7.65 mg/m ³ ⁱ 1 mg/m ³ = 0.13 ppm	1 ppm = 7.65 mg/m ³ ⁱ 1 mg/m ³ = 0.13 ppm
Explosive limits	No data	An explosive solid	No data	Moderate explosion hazard exposed to heat ⁱ

Table 3-2. Physical and Chemical Properties of Dinitrophenols (continued)

Property	3,4-Dinitrophenol	3,5-Dinitrophenol	Dinitrophenol mixture
Molecular weight	184.1	184.1	184.1
Color	Pale brown ^b	Colorless ^b	Yellow ^c
Physical state	Solid ^b	Solid ^b	Solid ^c
Melting point	134 °C ^b	122–123 °C ^b	No data
Boiling point	No data	No data	No data
Density (g/cm ³)	1.672 ^b	1.702 ^b	No data
Odor	No data	No data	No data
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Dissociation constant (pK _a)	5.42 ^d	3.68 ^b	No data
Solubility:			
Water at 18 °C	No data	No data	No data
Water at 35–36 °C	230 mg/L ^b	160 mg/L ^b	No data
Organic solvent(s)	No data	No data	Soluble in alcohol, ether, benzene, and chloroform ^c
Partition coefficients:			
Log K _{ow}	No data	2.36 ^g	No data
Log K _{oc}	No data	No data	No data
Vapor pressure	No data	No data	No data
Henry's law constant at 20 °C	No data	No data	No data
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 at 20 °C	1 ppm = 7.65 mg/m ³ ⁱ 1 mg/m ³ = 0.13 ppm	1 ppm = 7.65 mg/m ³ ⁱ 1 mg/m ³ = 0.13 ppm	1 ppm = 7.65 mg/m ³ ⁱ 1 mg/m ³ = 0.13 ppm
Explosive limits	No data	No data	Severe explosion hazard when dry ^c

^aMerck 1989^bHarvey 1959^cSax and Lewis 1987^dPearce and Simkins 1968^eMabey et al. 1981^fSchwarzenbach et al. 1988^gHansch and Leo 1985^hEstimated valueⁱHSDB 1994

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TABLE 3-3. Metabolites of Dinitrophenols

Parent	Metabolite	Metabolite	Metabolite
2,3-dinitrophenol 66-56-8*	2-amino-3-nitrophenol (3-nitro-2-aminophenol) 603-85-0	3-amino-2-nitrophenol (2-nitro-3-aminophenol) 14703-71-0	2,3-diaminophenol —
2,4-dinitrophenol 51-28-5	2-amino-4-nitrophenol ^a (4-nitro-2-aminophenol) 99-57-0	4-amino-2-nitrophenol ^a (2-nitro-4-aminophenol) 119-34-6	2,4-diaminophenol 95-86-3
2,5-dinitrophenol 329-71-5	2-amino-5-nitrophenol ^a (5-nitro-2-aminophenol) 121-88-0	5-amino-2-nitrophenol (2-nitro-5-aminophenol) 16292-86-7	2,5-diaminophenol —
2,6-dinitrophenol 573-56-8	2-amino-6-nitrophenol (6-nitro-2-aminophenol) 603-87-2	6-amino-2-nitrophenol ^b (2-nitro-6-aminophenol) 603-87-2	2,6-diaminophenol —
3,4-dinitrophenol 577-71-9	3-amino-4-nitrophenol (4-nitro-3-aminophenol) 16292-90-3	4-amino-3-nitrophenol (3-nitro-4-nitrophenol) 610-81-1	3,4-diaminophenol —
3,5-dinitrophenol 586-11-8	3-amino-5-nitrophenol (5-nitro-3-aminophenol) —	5-amino-3-nitrophenol ^b (3-nitro-5-aminophenol) —	3,5-diaminophenol —

* CAS number

^a Toxicity discussed in Chapter 2, Section 2.5.^b The aminonitrophenols in this row are chemically identical. The first entry is the preferred designation.

Alternate nomenclature for the aminonitrophenols is in parenthesis.