CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

DNPs are a class of synthetic organic chemicals that exist in six isomeric forms: 2,3-DNP, 2,4-DNP, 2,5-DNP, 2,6-DNP, 3,4-DNP, and 3,5 DNP. Information regarding the chemical identity of DNPs is located in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

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

Table 4-1. Chemical Identity of Isomers of Dinitrophenols[a]

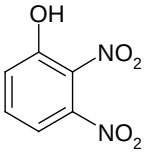
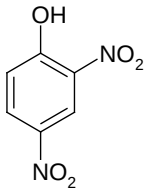
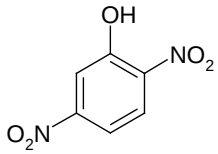
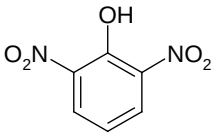
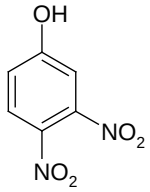
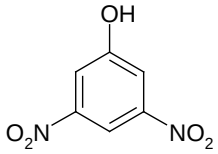
Characteristic	Information			
Chemical name	2,3-Dinitrophenol	2,4-Dinitrophenol	2,5-Dinitrophenol	2,6-Dinitrophenol
Synonym(s)	No data	1-Hydroxy-2,4-dinitrobenzene; α-Dinitrophenol; 2,4-DNP	γ-Dinitrophenol; 2,5-DNP[b]	β-Dinitrophenol[b]; 2,6-DNP
Registered trade name(s)	No data	Caswell No. 392; Sulfo Black B; Sulfo Black 2b Supra; Nitro Kleenup; others	No data	No data
Chemical formula	$C_6H_4N_2O_5$	$C_6H_4N_2O_5$	$C_6H_4N_2O_5$	$C_6H_4N_2O_5$
Chemical structure				
CAS Registry Number[c]	66-56-8	51-28-5	329-71-5	573-56-8

Table 4-1. Chemical Identity of Isomers of Dinitrophenols[a]

Characteristic	Information		
Chemical name	3,4-Dinitrophenol	3,5-Dinitrophenol	Dinitrophenol mixture
Synonym(s)	Δ-Dinitrophenol[c]; 4,5-Dinitrophenol[c]	θ-Dinitrophenol[c]	Dinitrophenol solution[c]
Registered trade name(s)	No data	No data	No data
Chemical formula	$C_6H_4N_2O_5$	$C_6H_4N_2O_5$	$(C_6H_4N_2O_5)$
Chemical structure			Usually a mixture of 2,3-, 2,4-, and 2,6- isomers
CAS Registry Number[c]	577-71-9	586-11-8	25550-58-7

[a]All information obtained from CHEMID (1992) and HSDB (1994), except where noted.
[b]RTECS 1992.
[c]SANSS 1992.

CAS = Chemical Abstracts Services

Table 4-2. Physical and Chemical Properties of Dinitrophenols

Property	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]	Yellow[a]
Physical state	Solid[b]	Solid[a]	Solid[a]	Solid[a]
Melting point	No data	Sublimes[a]	No data	No data
Boiling point	144°C[c]	112–114°C[a]	108°C[a]	63–64°C[a]
Density (g/cm^3)	1.681[c]	1.683[a]	No data	No data
Odor	No data	No data	No data	No data

Table 4-2. Physical and Chemical Properties of Dinitrophenols

Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility:				
Water (at 18°C)	No data	5,600 mg/L[d]	385 mg/L at 20°C[e]	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[f]	1.75[f]	1.37[f]
K_{oc}	No data	1.69[g,e]	No data	No data
pKa	4.89[b]	4.09[h]	5.22[h]	3.71[h]
Vapor pressure	No data	1.49×10^{-5} mmHg[d] at 18°C	1.05×10^{-3} mmHg[e] at 20°C	No data
Henry's law constant	No data	2.82×10^{-7} atm-m^3/mol[e,g]	6.61×10^{-7} atm-m^3/mol[e,g]	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	1 ppm=7.65 mg/m^3 [i] 1 mg/m3=0.13 ppm	1 ppm=7.65 mg/m^3 [i] 1 mg/m3=0.13 ppm	1 ppm=7.65 mg/m^3 [i] 1 mg/m3=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]

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

Table 4-2. Physical and Chemical Properties of Dinitrophenols

Odor	No data	No data	No data
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	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 solvents	No data	No data	Soluble in alcohol, ether, benzene, and chloroform[c]
Partition coefficients:			
Log K_{ow}	No data	2.36[f]	No data
K_{oc}	No data	No data	No data
pKa	5.42[h]	3.68[b]	No data
Vapor pressure	No data	No data	No data
Henry's law constant at 25°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 25ºC, 1 atmosphere)	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/m3=0.13 ppm	1 ppm=7.65 mg/m^3 [i] 1 mg/m3=0.13 ppm
Explosive limits	No data	No data	Severe explosion hazard when dry[c, j]

[a]Budavari et al. 1989.
[b]Harvey 1959.
[c]Sax and Lewis 1987.
[d]Mabey et al. 1981.
[e]Schwarzenbach et al. 1988.
[f]Hansch and Leo 1985.
[g]Estimated value.
[h]Pearce and Simkins 1987.
[i]HSDB 1994.
[j]WHO 2015.