# CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

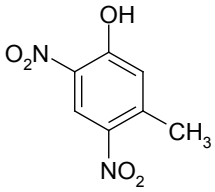
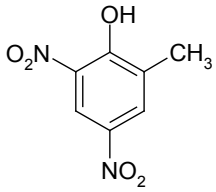
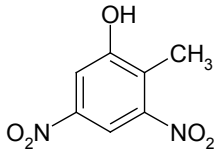
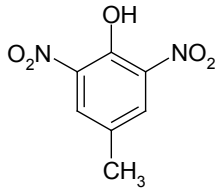
## 4.1 CHEMICAL IDENTITY

Table 4-1 lists common synonyms, trade names, and other pertinent identification information for selected dinitrocresols.

## 4.2 PHYSICAL AND CHEMICAL PROPERTIES

Table 4-2 lists important physical and chemical properties of dinitrocresols.

## Table 4-1. Chemical Identity of Dinitrocresols

| Chemical name | 4,6-Dinitro-*m*-cresol | 4,6-Dinitro-*o*-cresol[a] | 3,5-Dinitro-*o*-cresol | 2,6-Dinitro-*p*-cresol[a] |
|---|---|---|---|---|
| Synonym(s) and registered trade name(s) | 2,4-Dinitro-5-methylphenol; 3-methyl-4,6-dinitrophenol | DNOC; DNC; 3,5-dinitro-2-hydroxytoluene; 2-methyl-4,6-dinitrophenol; Antinonnin; Detal; Dinitrol; Effusan; Selinon; others[b] | 2-Methyl-3,5-dinitrophenol | DNPC; 3,5-dinitro-4-hydroxy toluene; Victoria Orange; Victoria Yellow |
| Chemical formula | $C_7H_6N_2O_5$ | $C_7H_6N_2O_5$ | $C_7H_6N_2O_5$ | $C_7H_6N_2O_5$ |
| Chemical structure |  |  |  |  |
| CAS Registry Number | 616-73-9 | 534-52-1 | 497-56-3 | 609-93-8 |

[a]All information obtained from ChemID 1993 and HSDB 1994 except where noted.
[b]Merck 1989.

CAS = Chemical Abstracts Service

## Table 4-2. Physical and Chemical Properties of Dinitrocresols

| Chemical name | 4,6-Dinitro-*m*-cresol | 4,6-Dinitro-*o*-cresol[a] | 3,5-Dinitro-*o*-cresol[b] | 2,6-Dinitro-*p*-cresol[c] |
|---|---|---|---|---|
| Molecular weight | 198.13 | 198.13 | 198.13 | 198.13 |
| Color | No data | Yellow | Yellow | Yellow |
| Physical state | No data | Solid | Solid | Solid |
| Melting point | No data | 87.5°C; 86.5°C[d] | 85.8°C | 80–81°C; 85°C[d] |
| Boiling point | No data | 312°C[e] | No data | No data |
| Density | No data | No data | 1.49 g/cm$^3$ [f] | No data |
| Odor | No data | Odorless[g] | No data | No data |
| Odor threshold: | | | | |
| Water | No data | No data | No data | No data |
| Air | No data | No data | No data | No data |
| $pK_a$ | No data | 4.46[h]; 4.38[i]; 4.35[j] | No data | No data |
| Solubility: | | | | |
| Water | No data | 130 mg/L at 15°C[k] | No data | 290 mg/L |
| Organic solvents | No data | Soluble in ethanol (4.3 g/100 g), acetone (100 g/100 g), and benzene (37 g/100 g)[g] | Soluble in ether, ethanol, and acetone[d] | Soluble in ether, ethanol, and acetone[d] |
| Partition coefficients: | | | | |
| Log $K_{ow}$ | No data | 2.12[l], 2.56[m], 2.16[i], 2.85[n] | No data | No data |
| Log $K_{oc}$ | No data | 2.35–2.77[a,o] | No data | No data |
| Vapor pressure | No data | 1.05x10$^{-4}$ mmHg at 25°C[p]<br>3.6x10$^{-4}$ mmHg at 35°C[r,s] | 5.2x10$^{-5}$ mmHg at 20°C[q] | No data |
| Henry's law constant | No data | 1.4x10$^{-6}$ atm-m$^3$/mol at 25°C[t,u] | No data | 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 |

## Table 4-2. Physical and Chemical Properties of Dinitrocresols

| | | | | |
|---|---|---|---|---|
| Conversion factors | 1 $mg/m^3$ = 0.12 ppm | 1 $mg/m^3$ = 0.12 ppm | 1 $mg/m^3$ = 0.12 ppm | 1 $mg/m^3$ = 0.12 ppm |
| Explosive limits | No data | No data | No data | No data |

[a]All information obtained from Merck 1989 unless otherwise noted.
[b]All information obtained from Lide 1993 unless otherwise noted.
[c]All information obtained from EPA 1988a unless otherwise noted.
[d]Lide 1993.
[e]ACGIH 1986.
[f]Bailey and White 1965 (no temperature value given).
[g]Metcalf 1978.
[h]Cessna and Grover 1978.
[i]Jafvert et al. 1990.
[j]Weber 1972.
[k]Meister 1991.
[l]Schwarzenbach et al. 1988.
[m]GEMS 1986.
[n]Loehr and Krishnamoorthy 1988.
[o]Kenaga 1980.
[p]Suntio et al. 1988.
[q]EPA 1979.
[r]Plimmer 1976.
[s]Hamaker and Kerlinger 1969.
[t]Shen 1982a.
[u]Shen 1982b.