

TOXICOLOGICAL PROFILE FOR  
4-AMINO-2,6-DINITROTOLUENE

Criteria and Standards Division  
Office of Drinking Water  
U.S. Environmental Protection Agency  
Washington, DC 20460

August 1989

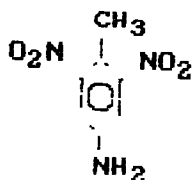
August 1989

TOXICOLOGICAL PROFILE  
FOR  
4-AMINO-2,6-DINITROTOLUENE

Criteria and Standards Division  
Office of Drinking Water  
U.S. Environmental Protection Agency  
Washington, DC 20460

## 4-AMINO-2,6-DINITROTOLUENE

### A. GENERAL

1. CAS Number: 19406-51-0
2. RTECS Number: XU6080000
3. General Name/Synonyms: 4-ADT  
4-Methyl-3,5-dinitroaniline  
4-Methyl-3,5-dinitrobenzenamine  
3,5-Dinitro-p-toluidine
4. Molecular Formula:  $C_7H_7N_3O_4$
5. Molecular Weight: 197
6. Structure:

### B. PHYSICAL AND CHEMICAL PROPERTIES

1. State: Yellow needles Buckingham and Donaghy (1982)
2. Vapor Pressure: No information was found.
3. Melting Point: 171°C Buckingham and Donaghy (1982)
4. Boiling Point: No information was found.
5. Specific Gravity: No information was found.
6. Solubility: No information was found.

7. Log  $K_{ow}$ : 1.06

Liu et al. (1983)

8. UV Absorption: No information was found.

#### C. PHYSICAL/CHEMICAL EQUILIBRIUM FACTORS:

1. Bioconcentration Factors (BCF): Liu et al. (1983) reported a steady-state BCF of 3.76 for 4-ADT; the value was based on an estimated log  $K_{ow}$ .

2.  $K_{wa}$ : No information was found.

3.  $K_{oc}$ : No information was found.

#### D. ENVIRONMENTAL FATE

1. Photolysis: Liu et al. (1983) demonstrated that 4-ADT (at a concentration of 1.8 mg/L of synthetic condensate wastewater) was readily and completely degraded by light. The wastewater sample was photoirradiated until a 44-mg/L concentration of 2,4-dinitrotoluene dropped to 10 mg/L ( $\pm 10\%$ ).

2. Leaching: No information was found.

3. Route of Water Contamination: No information was found.

4. Hydrolysis: No information was found.

5. Plant Uptake: No information was found.

6. Microbial Degradation: No information was found.

7. Persistence in Soil/Water: No information was found.

8. Byproducts: No information was found.

9. Vaporization: No information was found.

#### E. ACUTE TOXICITY IN MAMMALS

Animal/strain/sex	Route	LD <sub>50</sub> (mg/kg)	Reference
Mouse/CD-1/M	Oral	1342 ± 107 (1141-1611 mg/kg) <sup>a</sup>	Ellis et al. (1980)
F	Oral	1495 ± 90 (1318-1713 mg/kg)	
Rat/CD/M	Oral	1360 ± 53 (1260-1465 mg/kg)	Ellis et al. (1980)
F	Oral	959 ± 76 (787-1154 mg/kg)	

<sup>a</sup>95% confidence limits.

#### F. SKIN AND EYE IRRITATION AND SENSITIZATION IN MAMMALS

In a primary dermal and eye irritation study, 4-ADT (dose not specified) was nonirritating to the skin and eyes of rabbits (sex, strain, and number not reported) (Ellis et al., 1980).

In a sensitization study, no skin sensitization was observed in guinea pigs (sex, strain, and number not specified) exposed to 4-ADT (dose not specified) (Ellis et al., 1980).

#### G. SUBCHRONIC TOXICITY IN MAMMALS

No information was found.

#### H. REPRODUCTIVE EFFECTS AND TERATOGENICITY IN MAMMALS

No information was found.

#### I. MUTAGENICITY/GENOTOXICITY

Data are presented in tabular form on page 5.

#### J. CHRONIC/CARCINOGENICITY STUDIES IN MAMMALS

No information was found.

#### K. PHARMACOKINETICS IN MAMMALS

A single oral dose of <sup>14</sup>C-ring-labeled 4-ADT was readily absorbed and eliminated by CD albino rats (sex and number not given) (Ellis et al., 1980). The exact dosage was not specified, but the authors noted that animals were given approximately one-tenth of the LD<sub>50</sub> (i.e., 136 and 95.9/kg for males and females, respectively). Within 24 hours postdosing, about 40% of the administered radioactivity was recovered from the urine; 41% was found in the gastrointestinal tract and feces combined. The carcass contained about 2%.

Biliary excretion of  $^{14}\text{C}$ -ring-labeled 4-ADT by another group of rats was about 1 to 2% and 13% of the radioactive dose at 4 and 24 hours after administration of the test material, respectively (Ellis et al., 1980). The data from the biliary excretion study suggest that total absorption of 4-ADT is probably greater than the value reported in the first (i.e., oral dosing) study described above.

The biochemical effects of 4-ADT were examined by two groups of investigators. In one study, concentrations of  $10^{-12}$  to  $10^{-6}$  M 4-ADT had no effect on the synthesis of protein (globin) in cell-free extracts of reticulocytes from New Zealand white rabbits (Fournier and Parsons, 1980). In the second study, the activities of two heme synthesis regulatory enzymes, delta-aminolevulinic acid (the initial enzyme in heme production) and ferrochelatase (the final enzyme), remained unchanged in the presence of up to  $10^{-3}$  M 4-ADT. The test system included liver microsomes from male Walter Reed rats (Johnson et al. 1985).

#### L. HUMAN HEALTH EFFECTS

No information was found.

#### M. EXISTING STANDARDS/CRITERIA

No information was found.

# I. MUTAGENICITY/GENOTOXICITY

Test	Strain	Activation	Dose/concentration	Toxic effects	Reference
Ames mutagenicity assay	<u>Salmonella typhimurium</u> TA1535, TA1537, TA1538, TA98, TA100, TA100 NR3	± S9	10 to 5000 µg/plate	Positive both with and without activation in TA98 and TA100. Negative both with and without activation in TA1537 and TA100 NR3. In strain TA1535, positive with activation but negative without activation. In strain TA1538, positive without activation but negative with activation.	Spanggord et al. (1982)



## N. REFERENCES

Buckingham J, Donaghy SM. 1982. Dictionary of organic products. 5th ed. Vol. 4. New York: Chapman and Hall. p. 3827.

Ellis HV III, Hong C-B, Lee C-C. 1980. Mammalian toxicity of munitions compounds. Contract No. DAMD-17-74-C-4073. Environmental Protection Research Division. Available from: NTIS, Springfield, VA; ADA080146.

Fournier MJ, Parsons PP. 1980. The effects of specific environmental pollutants on the biosynthetic functions of mammalian cells in vitro. A search for structure/activity relationships. Contract Nos. DAMD-17-77-C-7044 and DAMD17-77-7045. Frederick, MD: U.S. Army Medical Research and Development Command. Available from: DTIC, Cameron Station, Alexandria, VA; ADA149184.

Johnson DJ, Williams HL, Slater S, Haut MJ, Alsfatt LB. 1985. The in vitro effects of selected environmental toxicants on two heme synthesis enzymes. J. Environ. Pathol. Toxicol. Oncol. 6:211-218.

Liu DHW, Bailey HC, Pearson JG. 1983. Toxicity of a complex munitions wastewater to aquatic organisms. ASTM Spec. Tech. Publ. 802:135-150.

Spanggord RJ, Mortelmans KE, Griffin AF, Simmon VF. 1982. Mutagenicity in Salmonella typhimurium and structure-activity relationships of wastewater components emanating from the manufacture of trinitrotoluene. Environ. Mutagen. 4:163-179.