

## Summary of Initial Risk Assessment Report

**Dinitrotoluene** CAS No : 25321-14-6

PRTR No of Japan: 157

This substance is assessed based on Guideline for Initial Risk Assessment Version 1.0

### 1. General Information

#### 1.1 Physico-chemical properties

Appearance	Yellow solid
Melting point	71 degC (2,4-type), 66 degC (2,6-type)
Boiling point	300 degC (2,4-type, degraded)
Water solubility	270 mg/L (2,4-type, 22 degC)
Henry's constant	$1.94 \times 10^{-8} \text{ Pa} \cdot \text{m}^3/\text{mol}$ ( $1.92 \times 10^{-13} \text{ atm} \cdot \text{m}^3/\text{mol}$ )* (25degC, estimated)
Octanol/water partition coefficient (log Kow)	1.98 (2,4-type, measured), 2.10 (2,6-type, measured) , 2.08**
Soil adsorption coefficient	Koc = 370 **(estimated)

\*\* the position of nitro group was not specified when estimation

#### 1.2 Environmental fate

Bioaccumulation	Exhibits little to no bioaccumulation Bioconcentration factor (BCF) : 0.6-2.9 (0.25 mg/L), 3.2-21.2 (0.025 mg/L) (carp) (measured)
Biodegradation	Non-biodegradable
Stability in the environment	(In air) Reaction with OH radical: Reaction rate constant is $2.2 \times 10^{-13} \text{ cm}^3/\text{molecule} \cdot \text{sec}$ (25 degC, estimated). The half-life is 2-3 months, given OH radical concentration of $5 \times 10^5 - 1 \times 10^6 \text{ molecule}/\text{cm}^3$ . Reaction with ozone: No data Reaction with nitrate radical: No data. (In water) Dinitrotoluene (hereinafter referred to as "DNT") is not hydrolyzed in aquatic environment.
Environmental fate	If released into water, DNT is expected to be dissolved in water and remain there. DNT is expected to be photodegraded near surface and part of it may be transferred to sediments. DNT may be removed by biodegradation under specific conditions involving acclimatized microorganisms.

### 2. Sources of release to the environment

#### 2.1 Annual production, import, export and domestic supply in 2001 (ton/year)

Production	Import	Export	Domestic supply	Remarks
--	--	--	232,500	

## 2.2 Uses

Chemical intermediates for toluenediamine (98.6%), raw materials for explosive/dyestuffs (1.4%)

## 2.3 Release from the industries within the scope of PRTR system (in 2001)

Release sources		Air (ton)	Waters (ton)	Soil (ton)	Remarks
Listed industries	Reported release	10	4	0	Release to rivers: 0 (release to sea only)
	Release outside notification	--	--	--	
Release outside notification from non listed industry		--	--	--	
Households		--	--	--	
Mobile sources		--	--	--	
Total		10	4	0	

## 2.4 Releases from other sources

No information about the substance is available.

## 2.5 Main release route

DNT is expected to be released into the environment mainly during production of toluenediamine, explosive intermediates, and dyestuffs those are made of DNT as a raw material.

### 3. Exposure Assessment

#### 3.1 Measured environmental concentration

Media	No. of points detected / No. of points measured	No. of samples detected / No. of samples measured	Detection range	95th percentile	Detection limit	Year of investigation, Institution
Air	--	--	--	--	--	--
River water (microg/L)	0/47	--	nd	--	0.01 <sup>1)</sup>	2000 Ministry of the Environment
Sea water (microg/L)	0/11	--	nd	--	0.01 <sup>1)</sup>	2000 Ministry of the Environment
Drinking water (as ground water) (microg/L)	0/15	--	nd	--	0.01 <sup>1)</sup>	2000 Ministry of the Environment
Food	--	--	--	--	--	--

nd: Not detected.

1) Sum of the values equal to 1/2 of detection limits of 2,4-DNT (0.01 microg/L) and 2,6-DNT (0.01 microg/L).

#### 3.2 Estimated environmental concentration

Media	Estimated concentration	Description
Air (microg/m <sup>3</sup> )	0.21	Calculated by mathematical model / Atmospheric Dispersion Model for Exposure and Risk Assessment ver.1.0 (AIST-ADMER), Maximum of annual average concentration.
River water (microg/L)	--	DNT was only released into sea water according to 2001 PRTR data. Concentration in river water was not estimated.

#### 3.3 Estimated environmental concentration in water (EEC)

EEC(microg/L)	0.01
	Sum of the values equal to 1/2 of the detection limits of 2,4-DNT (0.01 microg/L) and 2,6-DNT (0.01 microg/L) was used as the concentration in river.

### 3.4 Estimated human intake

Intake route		Concentration used for estimation of intake	Estimated intake (microg/ person/ day)	Estimated intake (microg/ kg-Bodyweight (BW)/ day)
Inhalation	Air	0.21 (microg/m <sup>3</sup> )	4.2	0.084
	Concentrations in air were unavailable. Estimated concentration of 0.21 microg/m <sup>3</sup> was used.			
Oral	Drinking water	0.01 (microg/L)	0.02	0.0004
	-Measured concentrations in tap water were unavailable. - Concentration in ground water was used as a substitute for that in tap water. -Sum (0.01 microg/L) of the values (0.005 microg/L) equal to 1/2 of the detection limits of 2,4-DNT and 2,6-DNT was used, since 2,4-DNT and 2,6-DNT were not detected in ground water.			
	Foods	0.00021 (microg/g)	0.025	0.0005
	-Measured concentrations of neither foods nor fish were available. -Concentration in fish was calculated as a product of a concentration in sea water and a BCF. -2,4-DNT and 2,6-DNT were not detected in sea water surveyed by the Ministry of the Environment. Therefore a sum (0.01 microg/L) of the values (0.005 microg/L) equal to 1/2 of detection limits of 2,4-DNT and 2,6-DNT was used. $0.01 \text{ (microg/L)} * 21.2 \text{ (L/kg)} \text{ (BCF)} = 0.00021 \text{ (microg/g)}$			
	Subtotal	--	0.045	0.0009
Total route		--	4.2	0.085

1) This substance is assessed based on the Guideline for Initial Risk Assessment Version 1.0. If adequate measured concentrations are available, they are given priority and used as values for risk assessment. If they are not available, an estimated value calculated using a mathematical model is used.

## 4. Hazard assessment

### 4.1 Effects on organisms in the environment

	Isomer	Acute or Chronic	Species	Endpoint	Concentration
Algae	2,4-DNT	Chronic	<i>Lemna minor</i>	96 hours NOEC Growth inhibition	0.32 (mg/L)
Crustacea	2,4-DNT	Chronic	<i>Daphnia magna</i>	21 days NOEC Reproduction	0.02 (mg/L)
Fish	2,4-DNT	Chronic	<i>Gasterosteus aculeatus</i>	35 days NOEC Growth	0.77 (mg/L)
Key study			The data of crustacea ( <i>daphnia magna</i> ) was chosen for the key study because effects were observed at the lowest concentration in the hazard assessment.		

## 4.2 Human health toxicity

Toxicity	Exposure route	Isomer	Species	Duration / Dose method	Toxic effects (Key study is underlined)	NOAEL or LOAEL
Repeated dose toxicity	Inhalation	--	--	--	--	--
	Oral	2,4-DNT	Dog (beagle)	2 years	<u>Anemia, hyperplastic liver foci</u> , atrophy of seminiferous tubules, decreased spermatogenesis, splenic pigmentation	NOAEL: 0.2 mg/kg/day
	Dermal	--	--	--	--	--
Reproductive and developmental toxicity	Oral	2,4-DNT	SD rat	Three-generation on reproduction toxicity test administration in feed	Low body weight and reduced survival rate in F2,F3 generations	NOAEL: 34.5 mg/kg/day
Carcinogenicity	Evaluation by IARC : -2,4-DNT and 2,6-DNT: Group 2B (possibly carcinogenic to humans) -2,3-DNT: Group 3 (not classifiable as to its carcinogenicity to humans) -DNT for industrial use (mixture): Not evaluated by IARC.					
Genotoxicity	-2,4-DNT, 2,6-DNT and DNT for industrial use are considered to be genotoxic. -2,5-DNT, 3,5-DNT are probably genotoxic.					

## 5. Risk Assessment

### 5.1 Environmental organisms

Risk characterization	EEC (microg/L)	NOEC * (mg/L)	MOE (NOEC * /EEC)	Product of uncertainty factors	Conclusion
	0.01	NOEC: 0.02	2,000	10	No immediate concern
Product of uncertainty factors (UF): Extrapolation from laboratory test (10) = 10					
Recommendation : The substance is considered to be of no immediate concern for the moment, and a low priority for further work.					

\* NOEC means NOEC, LOEC, EC<sub>50</sub>, etc.

## 5.2 Human health

### 5.2.1 Repeated dose toxicity

Exposure route	Intake (microg/kgBW/day)	NOAEL (mg/kgBW/day)	Risk characterization		
			MOE	Product of uncertainty factors	Conclusion
Inhalation	0.084	No adequate data	Not calculated	Not calculated	--
Oral	0.0009	0.2	220,000	100	No immediate concern
Total	0.085	0.2 (Oral )	2,400	100	No immediate concern
Product of uncertainty factors (UF): Oral/Total: Interspecies (10) * Intraspecies (10) = 100					

### 5.2.2 Reproductive and developmental toxicity

Since NOAEL of reproductive toxicity is larger than NOAEL of repeated dose toxicity, risk characterization of reproductive toxicity was not carried out.

### 5.2.3 Carcinogenicity

Risk characterization of carcinogenicity of the substance was not carried out in this assessment.

### 5.2.4. Recommendation

Although there was no adequate toxicity data available to evaluate exposure via the inhalation route, the MOE calculated using total intake from both routes (inhalation and oral) is larger than the product of uncertainty factors. Thus, the substance is considered to be of no immediate concern for the moment and a low priority for further work. It should be noted that a carcinogenic risk characterization was not conducted. The possibility remains that this substance may be carcinogenic to humans.

## 6. Supplement

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