12	CAS No.: 121-14-2	Substance: 2,4-Dinitrotoluene

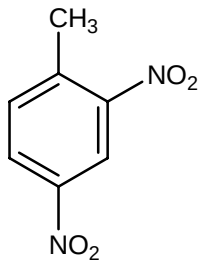
Chemical Substances Control Law Reference No.: 3-446 (as dinitrotoluene)

PRTR Law Cabinet Order No.: 1-157 (as dinitrotoluene)

Molecular Formula: $C_7H_6N_2O_4$

Molecular Weight: 182.14

Structural Formula:



1. General information

The aqueous solubility of this substance is 270 mg/L (22°C) and the partition coefficient (1-octanol / water) (log Kow) is 1.98. The vapor pressure is 1.32×10^{-4} mmHg (= 1.76×10^{-2} Pa) (20°C). Degradability (aerobic degradation) in terms of BOD-based degradation percentage is estimated to be 0%. The bioconcentration of this substance is thought to be zero or very low. In addition, this substance does not have hydrolyzable groups.

Dinitrotoluene is a Type 2 and Type 3 Monitoring Chemical Substance under the Law Concerning the Examination and Regulation of Manufacture, etc. of Chemical Substances and a Class 1 Designated Chemical Substance under the Law concerning Reporting, etc. of Releases to the Environment of Specific Chemical Substances and Promoting Improvements in Their Management (PRTR Law). It is used primarily as organic syntheses, a raw material of toluizine, dyes, and an intermediate compound of explosive. The quantity of production and import in FY2004 was 195 tons. The contents of Dinitrotoluene isomers in the general chemical products were approximately 75% for 2,4-Dinitrotoluene and approximately 20% for 2,6-Dinitrotoluene.

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2. Exposure assessment

Total release of Dinitrotoluene to the environment in FY2004 under the PRTR Law came to approximately 0.68 tons, all of which was reported. Release to the public water bodies accounted for a large part of the reported release. Chemical Industry accounted for all of the reported release.

The distribution into each environment medium predicted by means of a multimedia model was 87.0% for water bodies and 10.3% for bottom in the case of the region where the release quantity to the environment and public water bodies was considered to be the maximum. In the case of the region where the release quantity to the atmosphere was considered to be the maximum, the distribution was 86.5% for water bodies and 10.2% for bottom.

The predicted maximum exposure concentration for inhalation exposure to human beings was approximately 0.0011 μg/m^3. The predicted maximum oral exposure was estimated to be less than 0.0204 μg/kg/day.

The predicted environmental concentration (PEC) that indicates exposure to aquatic organisms was estimated to be less than 0.01 μg/L for freshwater and less than 0.01 μg/L for seawater public water bodies.

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3. Initial assessment of health risk

This substance causes irritation of the eyes and skin, and may have effects on CNS, cardiovascular system and blood, and may produce methemoglobin. The inhalation or ingestion may result in blue lips, nails and skin, headache, dizziness, nausea, confusion, convulsion, and unconsciousness. Contact to the skin may be absorbed and cause the similar symptoms. Contact to the eyes may result in redness.

There was insufficient information regarding the carcinogenicity of the substance. For this reason, an initial assessment of the substance was conducted based on information of non-carcinogenic effects.

As the 'Non-toxic level' for the oral exposure, the NOAEL of 0.2 mg/kg/day (neural toxicity, Heinz body red blood cells, biliary epithelial hyperplasia, etc.) was obtained from the medium- and long-term toxicity testing for dogs. For inhalation exposure, the 'Non-toxic level' could not be estimated.

With regard to oral exposure, in case of intakes of the groundwater and food, the predicted maximum exposure was approximately less than 0.02 μg/kg/day. The MOE of exceeding 200 was derived from the 'Non-toxic level' of 0.2 mg/kg/day divided by the predicted maximum dose, and divided by 10, because the 'Non-toxic level' was established by means of animal testing, and considering the carcinogenesis, it was further divided by 5. Accordingly, further action for assessment of its health risk from oral exposure to this substance would not be required at present.

For the inhalation, because its 'Non-toxic level' was not determined, its health risk could not be identified. Release to the atmosphere of this substance accounted for only 7% in the total release of Dinitrotoluene (reported quantity of release: 0.68 tons) and it is estimated that almost all of it is distributed into the media other than the atmosphere. As a reference, assuming that the absorption rate is 100 %, and the 'Non-toxic level' for the oral exposure is converted to the 'Non-toxic level' for the inhalation, the value is 0.67 mg/m^3. The MOE determined from this figure and the predicted maximum exposure concentration is 12,000. Accordingly, it would be low necessity of collecting information on inhalation exposure to this substance in the ambient air for its health risk assessment.

Information of toxicity				Exposure assessment		Result of risk assessment			Judgment
Exposure path	Criteria for risk assessment	Animal	Criteria for diagnoses (endpoint)	Exposure medium	Predicted maximum exposure quantity and concentration				
Oral	'Non toxic level' 0.2 mg/kg/day	Dogs	neural toxicity, Heinz body red blood cells, biliary epithelial hyperplasia, etc	Drinking water, food	– μg/kg/day	MOE	–	×	○
				Groundwate,food	< 0.02 μg/kg/day	MOE	> 200	○	
Inhalation	'Non toxic level' – mg/m^3	–	–	Ambient air	0.0011 μg/m^3	MOE	–	×	×
				Indoor air	– μg/m^3	MOE	–	×	×

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4. Initial assessment of ecological risk

With regard to acute toxicity, reliable information of a 48-hour EC_{50} growth inhibition value of 6,300 μg/L was found for the algae *Desmodesmus subspicatus*, a 48-hour EC_{50} immobilization value of 26,200 μg/L was found for the crustacea *Daphnia magna* (water flea), and a 96-hour LC_{50} value of 6,300 μg/L was found for the fish *Gasterosteus aculeatus* (threespine stickleback). Accordingly, an assessment factor of 100 was used, a predicted no effect concentration (PNEC) of 63 μg/L was obtained based on the acute toxicity values. With regard to chronic toxicity, reliable information of a 21-day NOEC reproduction value of 20 μg/L was found for the crustacea *D. magna*, and a 4-week NOEC growth inhibition value after hatching of 770 μg/L was found for the fish *G. aculeatus* (threespine stickleback). So an assessment factor of 100 was used, and a PNEC value of 0.20 μg/L was obtained based on the chronic toxicity values. As the PNEC for the substance, a value of 0.20 μg/L obtained from the chronic toxicity for the crustacea was used.

The PEC/PNEC ratio was less than 0.05 for both freshwater bodies and seawater bodies. Accordingly, further work is thought to be unnecessary at this time.

Hazard assessment (basis for PNEC)			Assessment factor	Predicted no effect concentration PNEC (μg/L)	Exposure assessment		PEC/ PNEC ratio	Result of assessment
Species	Acute / chronic	Endpoint			Water body	Predicted environmental concentration PEC (μg/L)		
Crustacea (water flea)	Chronic	NOEC reproduction	100	0.20	Freshwater	< 0.01	< 0.05	○
					Seawater	< 0.01	< 0.05	

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5. Conclusions

	Conclusions		Judgment
Health risk	Oral exposure	No need of further work.	○
	Inhalation exposure	Impossible of risk characterization. However, there is thought to be comparatively little need to collect information, etc.	×
Ecological risk	No need of further work.		○

［Risk judgments］ ○: No need of further work ▲: Requiring information collection
■: Candidates for further work ×: Impossible of risk characterization

Non-toxic level *

・When a LOAEL is available, it is divided by 10 to obtain a level equivalent to NOAEL.

・When an adverse effect level for the short-term exposure is available, it is divided by 10 to obtain a level equivalent to an adverse effect level for the long-term exposure.