4	CAS No.: 51-28-5	Substance: 2,4-Dinitrophenol

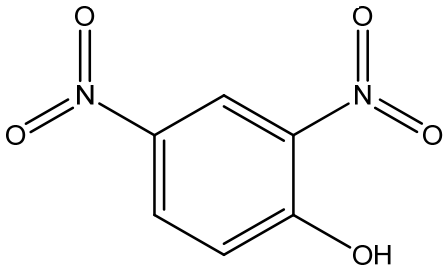
Chemical Substances Control Law Reference No.: 3-797 (2,4- Dinitrophenol (and its Na salts))

PRTR Law Cabinet Order No.:1-201

Molecular Formula: $C_6H_4N_2O_5$

Molecular Weight: 184.11

Structural Formula:



1. General information

The aqueous solubility of this substance is 690 mg/1,000 g (25°C), the partition coefficient (1-octanol/water) (log K_{ow}) is 1.67 (pH=1.5), and the vapor pressure is 5.10×10^{-3} mmHg (= 0.68 Pa) (20°C). The biodegradability (aerobic degradation) is characterized by a BOD degradation rate of 0%. Further, the substance does not possess any hydrolyzable groups.

This substance is designated as 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).

The main uses of this substance are as raw material for black dyestuffs used in blackout curtains and black denim, and as a polymerization inhibitor. The production and import quantity in fiscal 2015 was not disclosed because the number of reporting businesses was less than two. The production and import category under the PRTR Law is more than 100 t.

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2. Exposure assessment

Total release to the environment in fiscal 2015 under the PRTR Law was 0.057 t; all releases were reported. All reported releases were to public water bodies. In addition, approximately 41 t was transferred to waste materials. The chemical industry was the sole source of reported releases.

A multi-media model used to predict the proportions distributed to individual media in the environment indicated that in regions where the largest quantities were estimated to have been released to the environment overall or public water bodies in particular, the predicted proportion distributed water bodies was 97.8%.

Information to determine the maximum expected inhalation exposure could not be obtained. However, past general environmental atmospheric data, albeit surveyed for a limited area, indicated a maximum exposure of 0.015 μg/m^3.

The maximum expected oral exposure was estimated to be around 0.01 μg/kg/day based on calculations from data for public freshwater bodies. The maximum expected oral exposure calculated using public freshwater data for a limited area (0.72 μg/L) was 0.029 μg/kg/day. Further, an exposure of around less than 0.41 μg/kg/day was obtained taking into consideration data for exposure to public freshwater bodies (around 0.01 μg/kg/day) and food (around less than 0.4 μg/kg/day), although the latter data was from fiscal 1999. Further, in terms of food data, fiscal 2009 maximum concentrations for fish species (0.00012 μg/g) and shellfish species (0.00011 μg/g) were used along with average daily intakes of 66.6 g/capita/day for fish species and 2.4 g/capita/day for shellfish species to calculate an exposure by intake from an environmental medium via food of 0.0001 μg/kg/day. Combining this with the oral exposure estimated from public freshwater body data gives 0.01 μg/kg/day.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, was around 0.25 μg/L for public freshwater bodies and around 0.041 μg/L for seawater. Further, an environmental survey of public freshwater bodies covering a limited area reported a maximum value of 0.72 μg/L.

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3. Initial assessment of health risk

This substance may cause effects on metabolism, resulting in very high body temperature. Exposure may result in death. It causes nausea, vomiting, palpitation, collapse and sweating, if inhaled or ingested. Contact with the skin causes redness, roughness and yellow staining of the skin. The substance on the skin may be absorbed to cause nausea, vomiting and some other symptoms. The lowest lethal dose in humans is reported to be 36 mg/kg for oral exposure.

As sufficient information on the carcinogenicity of the substance was not available, the initial assessment was conducted on the basis of information on its non-carcinogenic effects.

The LOAEL for oral exposure of 2.0 mg/kg/day (based on cataract), determined from the effects observed in humans, was divided by a factor of 10 to account for extrapolation to chronic exposure, and by another factor of 10 to account for uncertainty in using a LOAEL. The calculated value of 0.02 mg/kg/day was deemed to be the lowest reliable dose and was identified as the 'non-toxic level*' of the substance for oral exposure. The 'non-toxic level*' for inhalation exposure could not be identified.

With regard to oral exposure, assuming the substance is absorbed via public freshwater bodies, the predicted maximum exposure level would be 0.01 μg/kg/day, approximately. The MOE (Margin of Exposure) would be 2,000, when calculated from the predicted maximum exposure level and the 'non-toxic level*' of 0.02 mg/kg/day. The predicted maximum exposure level would be less than 0.41 μg/kg/day, approximately, based on the concentrations in food as reported in 1999, and those in public freshwater bodies. The MOE derived from this exposure level would be more than 49. However, the predicted maximum exposure level would be 0.01 μg/kg/day when the exposure level via food is estimated from the concentrations in seafood, and the MOE derived from this exposure level would be 2,000. Therefore, no further work would be required at present to assess the health risk of this substance via oral exposure.

With regard to inhalation exposure, owing to the lack of identified 'non-toxic level*' and exposure levels, the health risk could not be assessed. The total release of the substance to the environment was reported to be 0.057 t in FY 2015 under the PRTR Law. However, the air emission of the substance was reported to be 0 t, and predictions of the multimedia fugacity model indicated that proportion distributed to air was little. In addition, assuming that 100% of the ingested substance is absorbed, the 'non-toxic level*' for inhalation exposure, derived from the conversion of the 'non-toxic level*' for oral exposure, would be 0.067 mg/m^3. The maximum exposure concentration in ambient air in a restricted area as reported in 2001 was 0.015 μg/m^3. The MOE would be 4,500, when calculated from this concentration and the converted 'non-toxic level*' for inhalation exposure. Therefore, collection of further information would not be required to assess the health risk of this substance via inhalation in ambient air.

Toxicity				Exposure assessment		Result of risk assessment			Judgment
Exposure Path	Criteria for risk assessment	Animal	Criteria for diagnoses (endpoint)	Exposure medium	Predicted maximum exposure dose and concentration				
Oral	'Non-toxic level*' 0.02 mg/kg/day	Humans	Cataract	Drinking water	— μg/kg/day	MOE	—	×	○
				Public Freshwater bodies	0.01 μg/kg/day	MOE	2,000	○	
Inhalation	'Non-toxic level*' — mg/m^3	—	—	Ambient air	— μg/m^3	MOE	—	×	(○)
				Indoor air	— μg/m^3	MOE	—	×	×

Non-toxic level *

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

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4. Initial assessment of ecological risk

With regard to acute toxicity, the following reliable data were obtained: a 96-h IC_{50} of 2,600 μg/L for growth inhibition in the green alga *Pseudokirchneriella subcapitata*, a 96-h LC_{50} of 3,080 μg/L for the crustacean *Gammarus pseudolimnaeus*, a 96-h LC_{50} of 390 μg/L for the fish species *Oncorhynchus mykiss* (rainbow trout), and a 24-h LC_{50} of 1,620 μg/L for the ciliate *Spirostomum ambiguus*. Accordingly, based on these acute toxicity values and an assessment factor of 100, a predicted no effect concentration (PNEC) of 3.9 μg/L was obtained.

With regard to chronic toxicity, the following reliable data were obtained: a 21-d NOEC of 2,000 μg/L for reproductive inhibition in the crustacean *Daphnia magna*, and a 60-d NOEC of 23 μg/L for growth inhibition in the fish species *Cirrhinus mrigala*. Accordingly, based on these chronic toxicity values and an assessment factor of 100, a PNEC of 2.3 μg/L was obtained.

The value of 2.3 μg/L obtained from the chronic toxicity to the fish species was used as the PNEC for this substance.

The PEC/PNEC ratio is 0.11 for freshwater bodies and 0.02 for seawater. Accordingly, efforts to collect data are needed. Further, an environmental survey of a limited area (public freshwater body) reported a PEC/PNEC ratio of 0.3. Regarding this substance, efforts are needed to understand trends in production and import quantities as well as in PRTR data, and the necessity of conducting a survey of prevalent concentrations in public water bodies should be considered.

Hazard assessment (basis for PNEC)			Assessment coefficient	Predicted no effect concentration PNEC (μg/L)	Exposure assessment		PEC/ PNEC ratio	Judgment based on PEC/PNEC ratio	Assessment result
Species	Acute/ chronic	Endpoint			Water body	Predicted environmental concentration PEC (μg/L)			
Fish *Cirrhinus mrigala*	Chronic	NOEC Growth inhibition	10	2.3	Freshwater	0.25	0.11	▲	▲
					Seawater	0.041	0.02		

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5. Conclusions

	Conclusions		Judgment
Health risk	Oral exposure	No need for further work.	○
	Inhalation exposure	Although risk to human health could not be confirmed, collection of further information would not be required.	(○)
Ecological risk	Requiring information collection.		▲

［Risk judgments］ ○: No need for further work ▲: Requiring information collection

■: Candidates for further work ×: Impossibility of risk characterization

（○）: Although risk to human health could not be confirmed, collection of further information would not be required.

（▲）: Further information collection would be required for risk characterization.