7	CAS No: 793-24-8	Substance: *N*-(1,3-Dimethylbutyl)-*N'*-phenyl-*p*-phenylenediamine

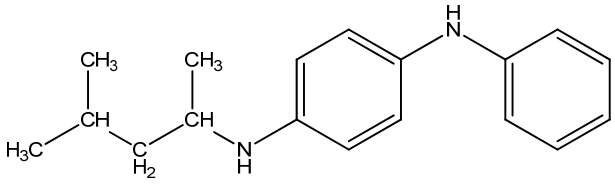
Chemical Substances Control Law Reference No.: 3-136 (*N*-alkyl(C3–9)-*N'*-phenyl-*p*-phenylenediamine), 3-368 (*N*-alkyl -*N'*-phenyl paraphenylenediamine (C3–10))

PRTR Law Cabinet Order: 1-230

Molecular Formula: $C_{18}H_{24}N_2$

Molecular Weight: 268.40

Structural Formula:



1. General information

The aqueous solubility of this substance is approximately 1 mg/L (50°C), the partition coefficient (1-octanol/water) (log K_{ow}) is 4.68 (calculated value), and the vapor pressure is 4.93×10^{-6} mmHg (= 6.57×10^{-5} Pa) (25°C, calculated value). Biodegradability (aerobic degradation) is characterized by a BOD degradation rate of approximately 2%, and bioaccumulation is thought to be low.

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 use of this substance is as a rubber antioxidant. The production quantity of *N*-alkyl(C3–9)-*N'*-phenyl-*p*-phenylenediamine in fiscal 2012 was 10,000 t, and that of *N*-alkyl-*N'*-phenyl paraphenylenediamine (C3–10) in fiscal 2012 was less than 1,000 t. 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 2012 under the PRTR Law was approximately 3.4 t, and all releases were reported. The sole destination of reported releases was the atmosphere. In addition, approximately 190 t was transferred to waste materials. The main source of reported releases was the rubber product manufacturing industry. 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 to the atmosphere in particular, the predicted proportion distributed to soil was 97.7%.

The maximum expected concentration of exposure to humans via inhalation, based on ambient air, was around 0.00024 μg/m^3. The mean annual value for atmospheric concentration in fiscal 2012 was calculated by using a plume-puff model on the basis of releases to the atmosphere reported according to the PRTR Law; this model predicted a maximum level of 1.1 μg/m^3. One report estimated the maximum expected oral exposure to be less than 0.000018 μg/kg/day on the basis of calculations from data for public freshwater bodies. The exposure level to this substance by intake from an environmental medium via food is considered slight, given the low bioaccumulation of the substance expected on basis of its physicochemical properties.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, was less than 0.00045 μg/L for public freshwater bodies and generally less than 0.00045 μg/L for seawater.

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3. Initial assessment of health risk

This substance causes slight irritation to the eyes and skin. Coughing may occur when inhaled. Contact of the substance with the skin and eyes may cause redness.

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

With regard to the oral exposure to the substance, the NOAEL of 4 mg/kg/day (based on hepatocellular steatosis and increase of the total serum proteins), obtained for mid-term and long-term toxicity tests on rats, was divided by a factor of 10 due to the short test periods. The outcome of 0.4 mg/kg/day was considered to be the reliable lowest dose of the substance and was identified as its 'non-toxic level*'. As for the inhalation exposure to the substance, the 'non-toxic level*' could not be established.

Regarding the oral exposure to the substance, the predicted maximum exposure was reported to be below 0.000018 μg/kg/day, assuming the ingestion of water from public water bodies and freshwater. The MOE of above 2,200,000 was derived from the substance's 'non-toxic level*' of 0.4 μg/kg/day and the maximum exposure level, after the division by a factor of 10 to convert animal data to human data. Therefore, no further action would be required at present to assess the health risk for the oral exposure to this substance.

Concerning inhalation exposure to the substance, the absence of information on the 'non-toxic level*'did not allow the assessment of the health risk. Nonetheless, assuming a 100 % absorption, and converting the 'non-toxic level*' for oral exposure to the inhalation one, the 'non-toxic level*' would be 1.3 mg/m^3. The MOE of 54,000 was derived from this level and the predicted maximum exposure concentration in ambient air of 0.00024 μg/m^3, and after the division by a factor of 10 to convert animal data to human data. In addition, the MOE of 120 was derived from the atmospheric maximum concentration of 1.1 μg/m^3 (annual mean) in high discharging plants areas, calculated from the reported emissions in FY 2012 under the PRTR Law. Therefore, collection of further information would not be required to assess the health risk for the inhalation exposure to this substance.

Toxicity				Exposure assessment			Result of risk assessment			Judgment
Exposure Path	Criteria for risk assessment	Animal	Criteria for diagnoses (endpoint)	Exposure medium	Predicted maximum exposure level and concentration					
Oral	'Non-toxic level*' 0.4 mg/kg/day	Rat	Hepatocellular steatosis and increase of the total serum proteins	Drinking water	–	μg/kg/day	MOE	–	×	○
				Freshwater	<0.000018	μg/kg/day	MOE	>2,200,000	○	
Inhalation	'Non-toxic level*' – mg/m^3	–	–	Ambient air	0.00024	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.

4.Initial assessment of ecological risk

With regard to acute toxicity, the following reliable data were obtained: a 96-h EC_{50} of 600 μg/L for growth inhibition in the green alga *Pseudokirchneriella subcapitata*, a 48-h EC_{50} of 230 μg/L for swimming inhibition in the crustacean *Daphnia magna*, and a 96-h LC_{50} of 28 μg/L for the fish species *Oryzias latipes* (medaka). Accordingly, based on these acute toxicity values and an assessment factor of 100, a predicted no effect concentration (PNEC) of 0.28 μg/L was obtained.

With regard to chronic toxicity, the following reliable data was obtained: a 41-d NOEC of 3.71 μg/L for growth inhibition in the fish species *O. latipes* (medaka). Accordingly, based on this chronic toxicity value and an assessment factor of 100, a PNEC of 0.037 μg/L was obtained.

The value of 0.037 μg/L obtained from the chronic toxicity to the crustacean was used as the PNEC for this substance.

The PEC/PNEC ratio is less than 0.01 for both freshwater bodies and seawater; accordingly, further work is

considered unnecessary at this time.

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 (medaka)	Chronic	NOEC Growth Inhibition	100	0.037	Freshwater	<0.00045	<0.01	○	○
					Seawater	<0.00045	<0.01		

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5. Conclusions

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

［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.