5	CAS No.: 624-92-0	Substance: Dimethyldisulfide

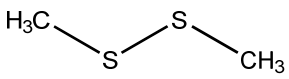
Chemical Substances Control Law Reference No.: 2-478

PRTR Law Cabinet Order No.: 1-219 (number after law revision*: 1-250)

Molecular Formula: $C_2H_6S_2$

Molecular Weight: 94.20

Structural formula:



1. General information

The aqueous solubility of this substance is approximately 2.7×10^3 mg/L (20°C) (pH≒6), the partition coefficient (1-octanol/water) (log K_{ow}) is 1.77, and the vapor pressure is 3,820 Pa (25°C). The biodegradability (aerobic degradation) is characterized by a BOD degradation rate of 0% and bioaccumulation is thought to be limited. Further, no hydrolyzation was reported in lake water (test duration: 108 days , 30°C).

This substance is classified as a Class 1 Designated Chemical Substance under the PRTR Law. The main uses of this substance are as a flavoring agent for onion and cabbage-based food products, as a raw material for organic synthesis, and as a first-stage catalyst for hydrogenation/desulfurization. Further, the production and import quantities in fiscal 2020 were not disclosed because the number of reporting businesses was less than two. The production and import category under the PRTR Law was more than 100 t.

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2. Exposure assessment

Total release to the environment in fiscal 2020 under the PRTR Law was approximately 0.20 t, and all releases were notified. The majority of notified releases to the atmosphere and public water bodies were to the atmosphere. In addition, 0.029 t was transferred to waste. The main notified release sources were the warehousing industry and the chemical 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 in general and the atmosphere in particular, the predicted proportion distributed to the atmosphere was 95.6%.

The maximum expected concentration of exposure to humans via inhalation could not be defined because ambient atmospheric and indoor air quality data could not be obtained. Further, the mean annual value for atmospheric concentration in fiscal 2020 was calculated by use of a plume-puff model on the basis of releases to the atmosphere reported under the PRTR Law: this model predicts a maximum level of 0.026 μg/m^3.

Data for potable water, groundwater, food, and soil to assess oral exposure could not be obtained. Thereupon, assuming ingestion solely from public freshwater bodies, a maximum predicted exposure of around 0.00064 μg/kg/day was obtained. Further, notified releases under the PRTR Law to public freshwater water bodies for fiscal 2020 were 0 kg, meaning concentrations in public water bodies originating from business sites that notify emissions are expected to be low. This substance is not judged to be highly bioaccumulative and as such, exposure from an environmental medium via ingestion is believed to be low.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, was around 0.016 μg/L for public freshwater bodies, and less than 0.0099 μg/L for seawater. Further, notified releases to public water bodies under the PRTR Law for fiscal 2020 were 0 kg, meaning concentrations in public water bodies originating from business sites that notify of emissions are expected to be low.

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3. Initial assessment of health risk

This substance irritates the respiratory tract, the eyes and the skin. Inhalation or ingestion of this substance will cause a

cough, sore throat, headache, nausea, dizziness, and drowsiness. Contact with the eyes will cause redness and pain. Contact with the skin will cause redness. The substance can be absorbed into the body through the skin and may cause headaches, nausea, etc.

Since not enough information was available on the carcinogenicity of the substance, the initial assessment was conducted based on information on its non-carcinogenic effects.

The 'non-toxic level' for oral exposure could not be identified. The NOAEL of 0.89 ppm (3.4 mg/m^3) for inhalation exposure (based on suppression of body weight gain), determined from toxicity tests in rats, was divided by a factor of 10 to account for extrapolation to chronic exposure. The calculated value of 0.34 mg/m^3 was deemed the lowest reliable concentration and was identified as the 'non-toxic level' of the substance for inhalation exposure.

Regarding oral exposure, due to the lack of an identified 'non-toxic level', the health risk could not be assessed. However, the tentative 'non-toxic level' of 0.10 mg/kg/day for oral exposure was derived from the conversion of the 'non-toxic level' for inhalation exposure, assuming that 100% of the ingested substance is absorbed. The MOE for reference would be 16,000 which is calculated from the tentative 'non-toxic level' for oral exposure and the predicted maximum exposure level of approximately 0.00064 μg/kg/day based on the data on public freshwater bodies, and subsequently divided by a factor of 10 to account for extrapolation from animals to humans. Since the release of this substance to public freshwater bodies was reported to be 0 kg in FY 2020 under the PRTR Law, the concentrations in public freshwater bodies derived from the effluents from the high discharging plants would not be high. In addition, since exposure to the substance in environmental media via food is presumed to be limited, despite the lack of exposure level via food, including it in the calculation would not change the MOE significantly. Therefore, as a comprehensive judgment, no further work would be required at present.

Regarding inhalation exposure, due to the lack of identified exposure concentrations, the health risk could not be assessed. However, the maximum concentration (annual mean) in ambient air near the operators that are releasing a large amount of the substance was estimated to be 0.026 μg/m^3, based on the releases to air reported in FY 2020 under the PRTR Law. The MOE for reference would be 1,300 which is calculated from the estimated concentration in ambient air and the 'non-toxic level' of 0.34 mg/m^3, and subsequently divided by a factor of 10 to account for extrapolation from animals to humans. Therefore, as a comprehensive judgment, the collection of further information would not be required to assess the health risk of this substance via inhalation in ambient air.

Toxicity				Exposure assessment		MOE		Comprehensive judgment
Exposure Path	Criteria for risk assessment	Animal	Criteria for diagnoses (endpoint)	Exposure medium	Predicted maximum exposure dose and concentration			
Oral	'Non-toxic level*' - mg/kg/day	-	-	Drinking water	- μg/kg/day	MOE	-	○
				Freshwater	0.00064 μg/kg/day	MOE	-	
Inhalation	'Non-toxic level*' 0.34 mg/m^3	Rats	Suppression of body weight gain, etc.	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 72-h of EC_{50} of 3,500 μg/L for growth inhibition in the cyanobacterium *Anabaena flos-aquae*, a 48-h EC_{50} of 1,610 μg/L for the crustacean *Daphnia magna*, and a 96-h LC_{50} of 960 μg/L for the fish *Oncorhynchus mykiss* (rainbow trout). Accordingly, based on these acute toxicity values and an

assessment factor of 100, a predicted no effect concentration (PNEC) of 9.6 μg/L was obtained.

With regard to chronic toxicity, the following reliable data were obtained: a 72-h NOEC of 170 μg/L for growth inhibition in the cyanobacterium *A. flos-aquae*, a 21-d NOEC of 2.5 μg/L for reproductive inhibition in the crustacean *D. magna*, and a 38-d NOEC of 473 μg/L for hatching rate, fry survival rate, and fry growth for the fish *Cyprinodon variegatus* (sheepshead minnow). Accordingly, based on these chronic toxicity values and an assessment factor of 10, a PNEC of 0.25 μg/L was obtained.

The value of 0.25 μg/L obtained from the chronic toxicity to the crustacean species was used as the PNEC for this substance.

The PEC/PNEC ratio was 0.06 for freshwater bodies and 0.04 for seawater.

Further work to assess the ecological risk of this substance is considered unnecessary at this time. Further, notified releases to public water bodies under the PRTR Law for fiscal 2020 were 0 kg, meaning concentrations in public water bodies originating from business sites that notify of releases were expected to be low. Accordingly, based on a comprehensive review of the above findings, 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	Comprehensive judgment
Species	Acute/ chronic	Endpoint			Water body	Predicted environmental concentration PEC (μg/L)		
Crustacean *Daphnia magna*	Chronic	NOEC Reproductive inhibition	10	0.25	Freshwater	0.016	0.06	○
					Seawater	0.0099	0.04	

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5. Conclusions

	Conclusions		Judgment
Health risk	Oral exposure	No need for further work.	○
	Inhalation exposure	No need for further work.	○
Ecological risk	No need for further work.		○

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

*Number after revision of law implemented on April 1, 2023