6	CAS No.: 132-65-0	Substance: Dibenzo [*b*,*d*] thiophene

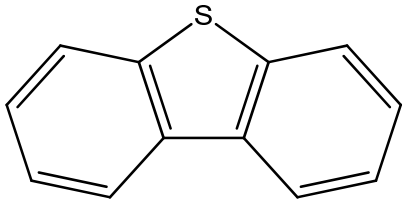
Chemical Substances Control Law Reference No.: 5-3352

PRTR Law Cabinet Order No.:

Molecular Formula: $C_{12}H_8S$

Molecular Weight: 184.26

Structural Formula:



1. General information

The aqueous solubility of this substance is 1.03 mg/1,000g (25℃), the partition coefficient (1-octanol/water) (log K_{ow}) is 4.38, and the vapor pressure is 2.04×10^{-6} mmHg (=2.72×10^{-4} Pa) (25℃). The biodegradability (aerobic degradation) is characterized by a BOD degradation rate of 0%, and bioaccumulation is thought to be nonexistent or low.

Moreover, hydrolyzation is not considered to be an important degradation pathway.

The main use of this substance is as a pharmaceutical intermediate. This substance is found in heavy oil and diesel. Coal tar creosote contains this substance (0.73–1.0 weight%).

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2. Exposure assessment

Because this substance is not classified as a Class 1 Designated Chemical Substance under the PRTR Law, release and transfer quantities could not be obtained. Predictions of proportions distributed to individual media by using a Mackay-type level III fugacity model indicated that if equal quantities were released to the atmosphere, water bodies, and soil, the proportion distributed to soil would be largest.

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 generally 0.052 μg/m^3.

The maximum expected oral exposure was estimated to be around 0.00016 μg/kg/day based on calculations from data for public freshwater bodies. Further, a daily exposure of around 0.011 μg/kg/day was also calculated from past data for public freshwater bodies as well as past data for soil in a study covering a limited area.

Data related to food could not be obtained. Therefore, recent (fiscal 2008) maximum concentrations for fish species (0.00063 μg/g) and shellfish species (0.0013 μg/g) were used along with average daily intakes (66.6 g/capita/day for fish species and 2.4 g/capita/day for shellfish species) to calculate an oral exposure via food of 0.0009 μg/kg/day. Combining this with the oral exposure estimated from public freshwater body data gives 0.0011 μg/kg/day.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, was around 0.0039 μg/L for public freshwater bodies and around 0.0023 μg/L for seawater. Further, a value of around 0.02 μg/L was reported in past data for public freshwater bodies and seawater.

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3. Initial assessment of health risk

No information was available on acute symptoms in humans. Abnormal behaviors including a general sluggishness was observed in mice exposed to this substance by ingestion. Full anesthesia with loss of righting reflex and of responses to tactile stimuli was observed in mice that received more than 325 mg/kg, which returned to normal within 24 hours. Mice that received more than 1,600 mg/kg remained comatose until death.

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 NOAEL for oral exposure of 3 mg/kg/day (based on increase in relative weight of the liver and kidneys, decrease in locomotor activity, etc.), determined from medium-term toxicity tests in rats, was divided by a factor of 10 to account for extrapolation to chronic exposure. The calculated value of 0.3 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 0.00016 μg/kg/day, approximately. The MOE (Margin of Exposure) would be 190,000, when calculated from the predicted maximum exposure level and the 'non-toxic level*'of 0.3 mg/kg/day, and subsequently divided by a factor of 10 to account for extrapolation from animals to humans.

Based on the concentrations in public freshwater bodies reported in 2006 and those in soil in a restricted area in 1991, the estimated maximum exposure level was 0.011 μg/kg/day, and the MOE calculated from this level would be 2,700. In addition, assuming the substance is absorbed via public freshwater bodies and seafood in the context of unidentified exposure level via food, the maximum exposure level would be 0.0011 μg/kg/day, and the MOE calculated from this level would be 27,000. 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 concentrations, the health risk could not be assessed. 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 1 mg/m^3. The maximum exposure concentration in ambient air as reported in a restricted area in 1991 was 0.052 μg/m^3. The MOE would be 1,900, when calculated from this concentration and the converted 'non-toxic level*' for inhalation exposure, and subsequently divided by a factor of 10 to account for extrapolation from animals to humans. 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*' 0.3 mg/kg/day	Rats	Increase in relative weight of the liver and kidneys, decrease in locomotor activity etc.	Drinking water	— μg/kg/day	MOE	—	×	○
				Public Freshwater bodies	0.00016 μg/kg/day	MOE	190,000	○	
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 EC_{50} of 60 μg/L for growth inhibition in the alga *Eutreptiella* sp., a 48-h LC_{50} of 242 μg/L for the crustacean *Palaemonetes pugio* (grass shrimp), and a 96-h LC_{50} 150 μg/L for the fish species *Pagrus major* (red seabream). Accordingly, based on these acute toxicity values and an assessment factor of 100, a predicted no effect concentration (PNEC) of 0.6 μg/L was obtained.

With regard to chronic toxicity, the following reliable data were obtained: a 72-h NOEC of 250 μg/L for growth inhibition in the green alga *Pseudokirchneriella subcapitata*, a 21-d NOEC of 54 μg/L for reproductive inhibition in the

crustacean *Daphnia magna*, and a 40-d NOEC of 32 μg/L for growth inhibition in the fish species *Oryzias latipes* (medaka). Accordingly, based on these chronic toxicity values and an assessment factor of 10, a PNEC of 3.2 μg/L was obtained.

The value of 0.6 μg/L obtained from the acute toxicity to the algal species was used as the PNEC for this substance.

The PEC/PNEC ratio is 0.007 for freshwater bodies and 0.004 for seawater; accordingly, further work is considered unnecessary at this time. Furthermore, while no data has been reported within the past 10 years, there is an older report of around 0.02 μg/L for seawater, and the ratio of this value and PNEC is less than 0.1.

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)			
Alga *Eutreptiella* sp.	Acute	EC_{50} Growth inhibition	100	0.6	Freshwater	0.0039	0.007	○	○
					Seawater	0.0023	0.004		

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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	No need of 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.