6	CAS No.: 4016-24-4	Substance: 2-Sulfohexadecanoic acid 1-methylester sodium salt

Chemical Substances Control Law Reference No.:

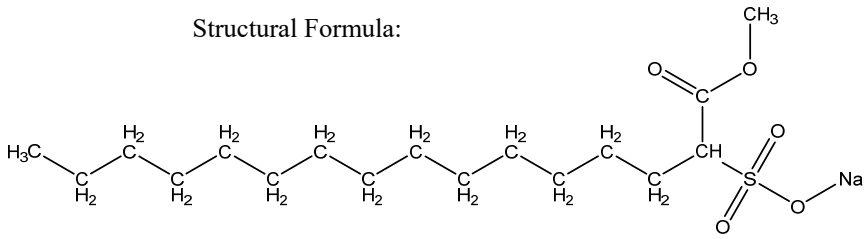
PRTR Law Cabinet Order No.: 1-24

Molecular Formula:

$C_{17}H_{33}NaO_5S$

Molecular Weight: 372.50

Structural Formula:



1. General information

The aqueous solubility of this substance is 271.9 mg/L (20°C, critical micelle concentration) and the vapor pressure is ≦ 1.3×10^{-4} mmHg (≦0.017 Pa) (100°C). The biodegradability (aerobic degradation) is characterized by a BOD degradation rate of 91–94%. Further, the substance does not hydrolyze (stable at pH of 4, 7, and 9 for 5 days at 50°C).

This substance is classified as a Class 1 Designated Chemical Substance under the PRTR Law. The main use of this substance is as a surfactant for laundry detergent. Japanese domestic production of this substance is 10,000–100,000 t/y, and production in 2001 was 13,400 t. The production and import quantity under the PRTR Law was over 100 t.

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2. Exposure assessment

Total release to the environment in fiscal 2017 under the PRTR Law was 0.002 t, and all releases were reported. All reported releases were to public water bodies, approximately 2.7 t was transferred to waste, and 0.0001 t was transferred to sewage. The chemical industry was the major reporter of 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 to water bodies was 79.4% and that to bottom sediment was 20.6%

The maximum expected concentration of exposure to humans via inhalation could not be determined because ambient atmospheric and indoor air quality data could not be obtained.

Data for potable water, ground water, public freshwater bodies, food, and soil to assess oral exposure could not be obtained. Further, albeit past data for a limited area, calculations for public freshwater bodies gave a daily exposure of 0.014 μg/kg/day. Conversely, when releases reported under the PRTR Law in fiscal 2017 to public freshwater bodies estimated from the reported transfer to public freshwater bodies were divided by the ordinary water discharge of the national river channel structure database, estimating the concentration in rivers by taking into consideration only dilution gave a maximum value of 0.011 μg/L. Calculating oral exposure based on this gives 0.00045 μg/kg/day. The risk of exposure to this substance by intake from an environmental medium via food is considered slight, given the low bioaccumulation of the substance expected on the basis of its physicochemical properties.

Data for setting the predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, could not be obtained. Further, past data indicated a maximum value of around 0.35 μg/L for public freshwater bodies. When releases reported under the PRTR Law in fiscal 2019 to public freshwater bodies estimated from the reported transfer to public freshwater bodies were divided by the ordinary water discharge of the national river channel structure database, estimating the concentration in rivers by taking into consideration only dilution gave a maximum value of 0.011 μg/L.

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3. Initial assessment of health risk

No information was available on acute symptoms in humans. Reduced locomotor activity was observed in rats immediately after oral administration of this substance. In these rats, ptosis and diarrhea were observed 1 to 3 hours after administration, followed by soiling of the perineal region by feces and urine and piloerection 3 to 6 hours after administration.

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 of 20 mg/kg/day for oral exposure (based on thickening of the mucosa and squamous hyperplasia in forestomach), determined from toxicity tests in rats, was divided by a factor of 10 to account for extrapolation to chronic exposure. The calculated value of 2.0 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, owing to the lack of identified exposure levels, the health risk could not be assessed. However, the MOE (Margin of Exposure) for reference would be 14,000, when calculated from the estimated maximum exposure level of 0.014 μg/kg/day and the 'non-toxic level' of 2.0 mg/kg/day, and subsequently divided by a factor of 10 to account for extrapolation from animals to humans. This maximum exposure level was estimated according to old data reported in 2004 on public freshwater bodies in a restricted area. Alternatively, the MOE for reference would be 440,000, when calculated from the estimated maximum exposure level of 0.00045 μg/kg/day. This maximum exposure level was estimated according to the concentration in effluents from the high discharging plants reported in FY 2017 under the PRTR Law. Since exposure to the substance in environmental media via food is presumed to be limited in spite of data unavailability, including it in the calculation would not change the MOE significantly. Therefore, as a comprehensive judgment, collection of further information would not be required 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. The total release of the substance into the environment was reported to be 0.002 t in FY 2017 under the PRER Law. However, the release of the substance into the air was reported to be 0 t, and predictions of the multimedia fugacity model indicated that the proportion distributed to air was little. Therefore, as a comprehensive judgment, 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	MOE		Comprehensive judgment
Oral	'Non-toxic level' 2.0 mg/kg/day	Rats	Thickening of the mucosa and squamous hyperplasia in forestomach	Drinking water	- μg/kg/day	MOE	-	○
				Groundwater	- μg/kg/day	MOE	-	
Inhalation	'Non-toxic level' - mg/m^3	-	-	Ambient air	- $\mu g/m^3$	MOE	-	○
				Indoor air	- $\mu g/m^3$	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 EC_{50} exceeding 9000 μg/L for growth inhibition in the green alga *Raphidocelis subcapitata*, a 48-h EC_{50} of 1240 μg/L for swimming inhibition in the crustacean *Daphnia magna*, and a 96-h LC_{50} of 1500 μg/L 7 μg/L for the fish *Oryzias latipes* (medaka). Accordingly, based on these acute toxicity values and an assessment factor of 100, a predicted no effect concentration (PNEC) of 12 μg/L was obtained.

With regard to chronic toxicity, the following reliable data were obtained: a 72-h NOEC of 1480 μg/L for growth inhibition in the green alga *R. subcapitata* and a 21-d NOEC of 240 μg/L for reproductive inhibition in the crustacean *D. magna*. Accordingly, based on these chronic toxicity values and an assessment factor of 100, a PNEC of 2.4 μg/L was obtained

The value of 2.4 μg/L obtained from the chronic toxicity to the crustacean was used as the PNEC for this substance.

Data for setting the predicted environmental concentration (PEC) could not be obtained for this substance. Accordingly, an assessment of ecological risk could not be made.

When releases reported under the PRTR Law in fiscal 2019 to public freshwater bodies estimated from the reported transfer

to public freshwater bodies were divided by the ordinary water discharge of the national river channel structure database, estimating the concentration in rivers by taking into consideration only dilution gave a maximum value of 0.011 μg/L, and the ratio of this value to the PNEC was 0.005. However, albeit data for a limited area of public water bodies, a maximum value of around 0.35 μg/L was reported and the ratio of this value to the PNEC was 0.15. Based on a comprehensive review of the above findings, efforts to collect data are needed, and environmental concentration data need to be augmented taking into consideration major emission sources and trends for production and import.

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	100	2.4	Freshwater	—	—	▲
					Seawater	—	—	

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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	Requiring information collection.		▲

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