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CAS No. 112-18-5

Substance: *N,N*-Dimethyldodecylamine

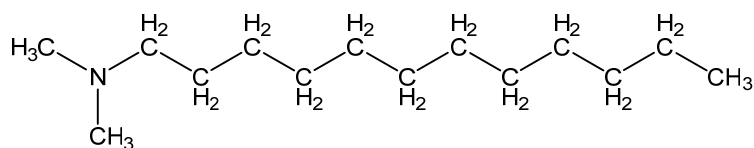
Chemical Substances Control Law Reference No.: 2-176 (*N,N,N*-Trialkyl (or alkenyl, at least one of the alkyl or alkenyl group is C8-24, others are H or C1-5) amine)

PRTR Law Cabinet Order No.: 223

Structural formula:

Molecular Formula: C₁₄H₃₁N

Molecular Weight: 213.40



1. General information

The aqueous solubility of this substance is 37 mg/L (20°C), the partition coefficient (1-octanol/water) (log Kow) is 5.44 (estimated value), and the vapor pressure is 2.1 Pa (25°C) (estimated value). The biodegradability (aerobic degradation) is characterized by a BOD degradation rate (NH₃) of 74%, and biodegradability is judged to be good. Further, this substance does not contain any hydrolyzable groups and as such, it does not undergo hydrolysis under ambient environmental conditions.

From the perspectives of ecological effects, this substance is designated as a Priority Assessment Chemical under the Chemical Substances Control Law and is also designated as a Class 1 Chemical Substance under the PRTR Law. The main uses of this substance are as a cationic surfactant, amphoteric surfactant, resin treatment agent, oil recovery agent, disinfectant, amine oxide, raw material for quaternary ammonium salts, flotation agent, pigment surface treatment agent, pigment flushing agent, fertilizer anti-caking agent, and textile softening agent. The production and import quantity in fiscal 2022 was 5593 t.

2. Exposure assessment

Total release to the environment in fiscal 2022 under the PRTR Law was approximately 0.005 t, and almost all releases were notified. The majority of notified releases were to the atmosphere. In addition, approximately 0.002 t was transferred to sewage and approximately 0.15 t was transferred to waste materials. The source of notified releases was 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 overall or to the atmosphere in particular, the predicted proportion distributed to the atmosphere would be 61.8%, and the predicted proportion distributed to soil would be 34.8%. Where the largest quantities were estimated to have been released to water bodies, the predicted proportion distributed to water was 68.7% and the predicted proportion distributed to sediment would be 30.5%.

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 2022 was calculated by use of a plume-puff model on the basis of releases to the atmosphere notified under the PRTR Law for fiscal 2022 and the model predicted a maximum level of 0.00069 µg/m³. Releases to the atmosphere under the PRTR Law vary from year to year. For this reason, an assessment was carried out erring on the side of caution using data from fiscal 2018, representing a recent year for which releases were at a high level. This gave a maximum predicted atmospheric concentration of 0.081 µg/m³.

Data for potable water, ground water, public freshwater bodies, food, and soil to assess oral exposure could not be obtained. Thereupon, assuming ingestion solely from public freshwater bodies, a maximum predicted daily exposure of around 0.048 µg/kg/day was obtained. Further, all notified releases of 0.2 kg to public water bodies in fiscal 2022 under the PRTR Law were to the sea, while the transfer ratio from sewage to public water bodies was 0%. Based on this scenario, the concentrations in public freshwater bodies originating from discharging business establishments is considered to be low. The 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. The 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.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, was around 1.2 µg/L for public freshwater bodies and around 0.003 µg/L for seawater. Further, all notified releases of 0.2 kg to public water bodies in fiscal 2022 under the PRTR Law were to seawater areas, while the transfer ratio from sewage to public water bodies was 0%. Based on this scenario, the concentrations in public freshwater bodies originating from discharging business establishments is not considered to be high.

3. Initial assessment of health risk

This substance severely irritates the skin and the eyes. While no information was available on acute toxicity of this substance in humans, severe corrosive effects were observed in rabbits after dermal application of the technical products (Genamin 12R 302D, Genamin LA 302D) of this substance for either three minutes or four hours in the acute dermal irritation/corrosion tests in accordance with the OECD test guideline 404.

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 NOAEL of 50 mg/kg/day for oral exposure (based on the behavior of rubbing a snout in bedding material observed immediately after administration of this substance), determined from a toxicity test in rats, was divided by a factor of 10 to account for extrapolation to chronic exposure. The calculated value of 5 mg/kg/day was deemed the lowest reliable dose and was identified as the ‘non-toxic level’ of the substance for oral exposure. Another study in rats provided the NOAEL of 50 mg/kg/day (based on the mortality of dams during pregnancy or lactation, influence on delivery or brooding care, increase in post-implantation loss, decrease in the number of pups delivered alive, etc.) as well. The ‘non-toxic level’ for inhalation exposure could not be identified.

Regarding oral exposure, assuming that the substance is absorbed via public freshwater bodies, the predicted maximum exposure level was approximately 0.048 µg/kg/day. The MOE (Margin of Exposure) would be 10,000 which is calculated from the predicted maximum exposure level and the ‘non-toxic level’ of 5 mg/kg/day and subsequently divided by a factor of 10 to account for extrapolation from animals to humans. This would lead to the health risk judgment that no further work would be required at present. Since the release of this substance to public water bodies was reported to be 0.2 kg, all of which was released into the sea, in FY 2022 under the PRTR Law, and the proportion of this substance in the sewage system transferred to public water bodies was determined to be 0%, the concentrations of this substance in public freshwater bodies derived from the discharging operators would not be high. In addition, exposure to this substance in environmental media via food is presumed to be limited despite the lack of exposure level via food, because high bioconcentration cannot be inferred from its physical and chemical properties. Including these exposures in the calculation would not change the MOE significantly. Therefore, as a comprehensive judgment, the collection of further information would not be required to assess the health risk of this substance via oral exposure.

Regarding inhalation exposure, due to the lack of identified ‘non-toxic level’ and exposure concentrations, the health risk could not be assessed. However, the tentative ‘non-toxic level’ for inhalation exposure of 17 mg/m³ was derived from the conversion of the ‘non-toxic level’ for oral exposure, assuming that 100% of the inhaled substance is absorbed. The maximum concentration (annual mean) in ambient air near the operators that are releasing a large amount of the substance was estimated to be 0.00069 µg/m³ based on the releases into air reported in FY 2022 under the PRTR Law. The MOE for reference would be 2,500,000 which is calculated from the estimated maximum concentration (annual mean) in ambient air and the tentative ‘non-toxic level’ of 17 mg/m³ and subsequently divided by a factor of 10 to account for extrapolation from animals to humans. When the maximum concentration in ambient air was estimated in the same way as the above using the data in FY 2018 when the release into air was highest in recent years in order to make a conservative assessment considering

the yearly fluctuation in the releases into air under the PRTR Law, it would be 0.081 µg/m³, giving an MOE of 21,000. 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		Result of risk assessment		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'	5	mg/kg/day	Rats	The behavior of rubbing a snout in bedding material immediately after administration	Drinking water	—	µg/kg/day	MOE	—	○
						Freshwater	0.048	µg/kg/day	MOE	10,000	
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.

4. Initial assessment of ecological risk

With regard to acute toxicity, the following reliable data were obtained: a 72-h EC₅₀ of 23.5 µg/L for growth inhibition in the green alga *Desmodesmus subspicatus*, a 48-h EC₅₀ of 83 µg/L for swimming inhibition in the crustacean *Daphnia magna*, and a 96-h LC₅₀ of 570 µg/L for the fish *Oncorhynchus mykiss* (rainbow trout). Accordingly, based on this acute toxicity value and an assessment factor of 100, a predicted no effect concentration (PNEC) of 0.23 µg/L was obtained.

With regard to chronic toxicity, the following reliable data were obtained: a 72-h NOEC of 2.6 µg/L for growth inhibition in the green alga *D. subspicatus*, a 21-d NOEC of 36 µg/L for reproductive inhibition in the crustacean *D. magna*, and a 48-h EC₂₀ of 97 µg/L for reproductive inhibition in the rotifer *Brachionus calyciflorus*. Accordingly, based on this chronic toxicity value and an assessment factor of 100, a predicted no effect concentration (PNEC) of 0.026 µg/L was obtained.

The value of 0.026 µg/L obtained from the chronic toxicity to the alga was used as the PNEC for this substance.

The PEC/PNEC ratio is 46 for freshwater bodies and 0.1 for seawater. Accordingly, this substance is considered a candidate for detailed assessment of ecological risk.

Total releases under the PRTR Law have exhibited a downward trend since the last assessment (14th Edition). In the 2017 water quality survey conducted after the 2013 survey used for the PEC, the maximum value was 0.19 µg/L, resulting in a ratio of 7 compared to the PNEC of 0.026 µg/L. Multiple locations exceeded the PNEC. In addition, while transfers to public water bodies and sewage were reported, information that could lead to identification of release sources to water could not be obtained.

Accordingly, this substance is considered a candidate for detailed assessment of ecological risk.

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)		
Green algae	Chronic	NOEC Growth inhibition	100	0.026	Freshwater	1.2	46	■
					Seawater	0.003	0.1	

5. Conclusions

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

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