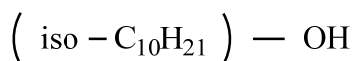| 2	CAS No.: 25339-17-7	Substance: Isodecyl alcohol

Chemical Substances Control Law Reference No.: 2-217 (Alkanols (C=5–38))

PRTR Law Cabinet Order No.: 1-257 （Decyl alcohol）

Molecular Formula: $C_{10}H_{22}O$

Molecular Weight: 158.28

Structural Formul[a)]:

$$\left(\text{iso} - C_{10}H_{21} \right) - OH$$

Note: a) Under IUPAC nomenclature, iso- is limited to a methyl group attached to the end of the alkyl group (i.e., 8-methylnonan-1-ol) but here, decyl alcohols for which the structure is not completely identified and a branched decyl group is the main constituent are referred to.

1.General information

The aqueous solubility of this substance is 96 mg/L (20°C), the partition coefficient (1-octanol/water) (log K_{ow}) is 3.94, and the vapor pressure is 2.07×10^{-2} mmHg (=2.76 Pa) (25°C). Biodegradability (aerobic degradation) is judged to be good (based on evaluation of a similar substance). Further, the substance does not possess any hydrolyzable groups and as such, it is not thought to hydrolyze under ambient environmental conditions.

Decyl alcohol is classified as a Class 1 Designated Chemical Substance under the PRTR Law. The main use of this substance is as a raw material for plasticizers (DIDP, DIDA) used in polyvinyl chloride resin-based wire encapsulation and high-quality leather seats. It is also used in uranium refining, defoaming agents, and as a raw material for surfactants. The production and import quantity of alkanols (C=5–38) in fiscal 2017 was 200,000 t. The production and import quantity under the PRTR Law of decyl alcohol was more than 100 t.

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2. Exposure assessment

Total release to the environment in fiscal 2017 under the PRTR Law was approximately 100 t, of which approximately 0.62 t was reported; thus, almost all releases were unreported. Further, approximately 70 t was transferred to waste and 0.032 t was transferred to sewage. The chemical industry was the main source of releases. The largest releases to the environment including unreported releases were to soil. A multimedia model used to predict the proportions distributed to individual media in the environment indicates that in regions where the largest quantities were estimated to have been released to the environment overall or soil in particular, the predicted proportion distributed to soil was 99.4%. Where the largest quantities were estimated to have been released to the atmosphere, the predicted proportion distributed to soil was 98.5%. Where the largest quantities were estimated to have been released to public water bodies, the predicted proportion distributed to water bodies was 94.5%.

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. The mean annual value for the atmospheric concentration of decyl alcohol in fiscal 2017 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 0.10 μg/m³ . Further, this estimate assumes that all reported releases of decyl alcohols are in the form of iso-decyl alcohol because overall reported releases of decyl alcohol including iso-decyl alcohol were all that could be obtained under the PRTR Law.

Data for potable water, ground water, public freshwater bodies, food, and soil to assess oral exposure could not be obtained. However, assuming all releases to public freshwater bodies in fiscal 2017 reported under the PRTR Law were iso-decyl alcohol, where these releases 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 2.0 μg/L. Using this estimated concentration for rivers to calculate oral exposure gives 0.080 μg/kg/day. Further, this estimate assumes that all reported releases of decyl alcohols are in the form of iso-decyl alcohol because overall reported releases of decyl alcohol including iso-decyl alcohol were all that could be obtained under the PRTR Law. In addition, when estimating river concentrations using reported releases, the maximum concentration in rivers that do not have environmental monitoring stations or supplementary monitoring points is 4.9 μg/L. Calculating oral exposure using this value gives 0.20

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. Assuming all releases to public freshwater bodies in fiscal 2017 reported under the PRTR Law were iso-decyl alcohol, where these releases 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 2.0 µg/L. In addition, when estimating river concentrations using reported releases, the maximum concentration in rivers that do not have environmental monitoring stations or supplementary monitoring points is 4.9 µg/L.

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3. Initial assessment of health risk

This substance is irritating to the respiratory tract, skin and eyes. Inhalation of the substance causes cough, dizziness, lethargy, headache, nausea and sore throat. Ingestion causes diarrhea and vomiting in addition to the same symptoms as inhalation. Contact with the skin causes dry skin and redness. Contact with the eyes causes redness and pain.

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 168 mg/kg/day for oral exposure (no observed effect dose), determined from toxicity tests in rats, was divided by a factor of 10 to account for extrapolation to chronic exposure. The calculated value of 17 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 8,500, when calculated from the estimated maximum exposure level of 0.20 µg/kg/day and the 'non-toxic level' of 17 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 the concentration in effluents from the high discharging plants reported as decyl alcohol 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. However, the MOE for reference would be 57,000, when calculated from the tentative 'non-toxic level' for inhalation exposure of 57 mg/m³ and the concentration in ambient air of 0.10 µg/m³, and subsequently divided by a factor of 10 to account for extrapolation from animals to humans. The tentative 'non-toxic level' for inhalation exposure above was derived from the conversion of the 'non-toxic level' for oral exposure, assuming that 100% of the inhaled substance is absorbed. The concentration in ambient air was estimated as the maximum concentration (annual mean) in ambient air near the operators releasing large amount of the substance based on the releases to air reported as decyl alcohol in FY 2017 under the PRTR Law. 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			
Oral	'Non-toxic level' 17 mg/kg/day	Rats	No observed effect dose	Drinking water	- µg/kg/day	MOE	-	○
				Groundwater	- µg/kg/day	MOE	-	
Inhalation	'Non-toxic level' - mg/m³	-	-	Ambient air	- µg/m³	MOE	-	○
				Indoor air	- µg/m³	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} of 6780 µg/L for growth inhibition in the alga *Raphidocelis subcapitata*, a 24-h TLm of 3400 µg/L for the crustacean *Artemia salina*, and a 96-h LC_{50} of 5870 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 34 µg/L was obtained.

With regard to chronic toxicity, the following reliable data were obtained: a 72-h NOEC of 1690 µg/L for growth inhibition in the alga *R. subcapitata*, and a 21-d NOEC of 400 µg/L for reproductive inhibition in the crustacean *D. magna*. Accordingly, based on this chronic toxicity value and an assessment factor of 100, a PNEC of 4 µg/L was obtained.

The value of 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.

Assuming that all releases to public water bodies reported in fiscal 2017 under the PRTR Law were in the form of iso-decyl alcohol, dividing by the ordinary water discharge of the national river channel structure database and estimating the concentration in rivers by taking into consideration only dilution gives a maximum value of 2.0 µg/L, and the ratio of this value to the PNEC is 0.5. In addition, when estimating river concentrations using reported releases, the maximum concentration in rivers that do not have environmental monitoring stations or supplementary monitoring points is 4.9 µg/L and the ratio of this value to the PNEC is 1.2; accordingly, based on a comprehensive review of the above findings, efforts to collect data are needed, and environmental concentration data needs to be augmented taking into consideration major emission sources.

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	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