1 CAS No.: 31093-47-7 (Decylbenzenesulfonic acid, C=10), 1322-98-1 (Benzenesulfonic acid, decyl, sodium. salt, C=10), 27636-75-5 (Undecylbenzenesulfonic acid sodium salt, C=11), 25155-30-0 (Dodecylbenzene sulfonic acid, sodium salt, C=12), 26248-24-8 (Tridecylbenzenesulfonic acid, sodium salt, C=13), 28348-61-0 (Tetradecylbenzenesulfonic acid, sodium salt, C=14), and others.

Substance: Linear alkyl benzenesulfonic acid and its salts

Chemical Substances Control Law Reference No.: 3-1884 (Normalalkyl (C6-14) benzenesulfonic acid and salt (K,Na,Li,Ca) thereof), 3-1906 (Salt (Na,K,Ca,Mg,Zn,Ba) of alkyl (C 6-16) benzenesulfonic acid), 3-1907 (Alkyl (C6-20) benzenesulfonic acid), 3-1949 (Salt (Ca,Na,K,Mg,Ba) of alkyl (C10-50) benzenesulfonate)

Structural Formula:

PRTR Law Cabinet Order No.: 1-24 Molecular Formula: $RC_6H_4SO_3X$ (R is an alkyl group with C_{10} to C_{14} ; X is

Na, etc.)

Molecular Weight: 348.48 (C₁₂Na)

$$H_3C$$
— $(CH_2)_j$ — C — $(CH_2)_k$ — CH_3
 $j+k=7 \sim 11$
 $X \text{ is Na, etc.}$

1. General information

The aqueous solubility of this substance is 300 mg/L (C_{12} Na, 20-25°C), and 2.0 x 10⁵ mg/L (C_{12} Na, 25°C), and the partition coefficient (1-octanol/water) (log Kow) is 1.96 (C_{12} Na) and 0.45 (C_{12} Na). The vapor pressure is 2.3 x 10⁻¹⁵ mmHg (C_{12} Na, 25°C, calculated value). Sodium alkylbenzenesulfonate (soft type) is determinated to be ready biodegradable.

This substance is a Class 1 Designated Chemical Substance under the Law concerning Reporting, etc. of Releases to the Environment of Specific Chemical Substances and Promoting Improvements in Their Management (PRTR Law). Approximately 80 percent of the substance is used for laundry detergent for home use, and a little less than 20 percent is used for cleaning agents for industrial use in general cleaning, kitchen cleaning, and car washing. Just a small amount is used for dispersants in fabric dyeing and finishing and emulsifiers for agricultural chemicals. It is rarely used for household kitchen detergents. Production of this substance in FY2005 came to 62,088 tons. The export quantity was 386 tons and the import quantity was 5,472 tons.

2. Exposure assessment

Total release to the environment in FY2005 under the PRTR Law came to approximately 14,000 tons, of which approximately 14,000 tons (over 99% of the total) was reported. Release to public water bodies accounted for a large part of the reported release. The transfers to sewage and waste were 17 and approximately 330 tons, respectively. Industries related to chemicals, textiles, and apparel, and other textile products reported large releases to public water bodies, and large releases to the air were reported by the chemical industry.

The largest reported releases to the environment were releases into water bodies, including estimated releases. This substance is a mixture in which alkyl chain length, the substituted position of the phenyl group on the alkyl chain, and the substituted position of the sulfone group are different. The ratio of distribution to each media was not estimated because of the unclear composition of the substance.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, was estimated to be approximately 1,100 μ g/L for freshwater and approximately 11 μ g/L for seawater public water bodies.

3. Initial assessment of ecological risk

With regard to acute toxicity, reliable information of a 96-hour median effective concentration (EC $_{50}$) population change value of 1,900 μ g/L was found for the diatom *Phaeodactylum tricornutum*, a 48-hour median lethal

concentration (LC₅₀) value of 370 μ g/L was found for the crustacea *Marsupenaeus japonicus* (kuruma shrimp), a 48-hour LC₅₀ value of 500 μ g/L was found for the fish *Ambassis commersoni* and a 96-hour LC₅₀ value of 1,660 μ g/L was found for another organism, the *Mytilus galloprovincialis*. Accordingly, an assessment factor of 100 was used, and a predicted no effect concentration (PNEC) of 3.7 μ g/L was obtained based on the acute toxicity values. With regard to chronic toxicity, a 72-hour no observed effect concentration (NOEC) for growth inhibition of the green algae *Pseudokirchneriella subcapitata* was 1,000 μ g/L, a 21-day NOEC for mortality and reproduction of the crustacea *Daphnia magna* was 570 μ g/L, a 263-day NOEC for reproduction inhibition of the fish *Pimephales promelas* (fathead minnow) was 106 μ g/L, and a 220-day NOEC for the filtration rate of the *Mytilus galloprovincialis* was 250 μ g/L. From these reliable data, a PNEC based on chronic toxicity was determined to be 11 μ g/L with an assessment factor of 10.

As the PNEC for the substance, a value of $3.7~\mu g/L$ obtained from the acute toxicity for the crustacea was used. The PEC/PNEC ratio was 300 for freshwater bodies and 3 for seawater bodies. This substance is thought to be a candidate for further work.

Hazard assessment (basis for PNEC)				Predicted no	Exposure assessment		PEC/	
Species	Acute / chronic	Endpoint	Assessment factor	effect concentration PNEC (μg/L)	Water body	Predicted environmental concentration PEC (μg/L)	PNEC ratio	Result of assessment
Crustacea	At -	LC ₅₀	100	2.7	Freshwater	1,100	300	
(kuruma shrimp)	Acute	mortality	100	3.7	Seawater	11	3	

4. Conclusions

	Conclusions	Judgment				
Ecological risk	Candidate for further work.	•				
[Risk judgments]	O: No need for further work ▲: Requiring information collection					
	■: Candidates for further work ×: Impossibility of risk characterization					
	(): Though a risk characterization cannot be determined, there would be little necessity					
	collecting information.					
	(): Further information collection would be required for risk characterization.					