CAS No.: 141-32-2 Substance: Butyl acrylate

Chemical Substances Control Law Reference No.: 2-989 (Alkyl acrylate (C=3-4))

PRTR Law Cabinet Order No.: - (Cabinet Order No. after revision*: 1-7)

Structural Formula:

Molecular Formula: C₇H₁₂O Molecular Weight: 128.17

*Note: No. according to revised order enacted on October 1, 2009.

1. General information

The aqueous solubility of this substance is 1.4×10^3 mg/L (20°C), the partition coefficient (1-octanol/water) (log Kow) is 2.36, and the vapor pressure is 5.48 mmHg (=731 Pa) (25°C). Biodegradability (aerobic degradation) is good.

Based on a revision of substances regulated by the Law Concerning Reporting, etc. of Releases to the Environment of Specific Chemical Substances and Promoting Improvements in Their Management (PRTR Law) (enacted on October 1, 2009), this substance was newly designated as a Class 1 Designated Chemical Substance. The main applications of acrylate esters are acrylic fiber, fiber processing, paints, paper processing, adhesives, leather processing, and acrylic rubber. The production (shipments) and import quantity in fiscal 2004 was 100,000 to <1,000,000 t, and the export quantity in fiscal 2004 was 9,380 t.

2. Exposure assessment

Because this substance was not classified as a Class 1 Designated Chemical Substance prior to revision of substances regulated by the PRTR Law, release and transfer quantities could not be obtained. Predictions of distribution by medium using a Mackay-type level III fugacity model indicated that if equal quantities were released to the atmosphere, water bodies, and soil, the proportions distributed to soil and water bodies would be higher.

Data for setting the predicted maximum exposure to humans via inhalation could not be obtained, but there is a report of $0.075~\mu g/m^3$ when data from a limited area (Tokyo Metropolis) was used. The predicted maximum oral exposure was estimated to be less than around $0.0004~\mu g/kg/day$ based on calculations from data for groundwater. The risk of exposure to this substance by intake from an environmental medium via food is considered slight.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, is less than around 0.01 µg/L for both public freshwater bodies and seawater.

3. Initial assessment of health risk

This substance is irritating to eyes, skin and respiratory tracts. When inhaled, it will cause burning sensation, coughing, short breaths and sore throat. When orally taken, it will cause abdominal pain, nausea, vomiting and diarrhea. When it contacts with eyes or skin, there will occur rubefaction or pain. Chemical pneumonia may occur when its liquid is swallowed and taken into lungs.

Sufficient information could not be obtained on its carcinogenicity, and its initial assessment was conducted on the basis of data on its non-carcinogenic effects.

As for its oral exposure, its no-observed-adverse-effect-level (NOAEL) of 84 mg/kg/day (for relative increase of liver weight to body weight) obtained from its mid-term and long-term toxicity tests for rats was divided by 10, due to their short test periods, to produce 8.4 mg/kg/day as its 'non-toxic level*'. As for its inhalation exposure, its LOAEL of 14 ppm (for atrophy/hyperplasia of olfactory epithelia) obtained from mid-term and long-term toxicity tests for rats was adjusted against exposure conditions to produce 2.5 ppm (13 mg/m³). Since this was LOAEL, it was then divided by 10

to provide 1.3 mg/m³ as its 'non-toxic level*'.

As for its oral exposure, its maximum exposure was estimated to be less than around $0.0004 \,\mu g/kg/day$, when intakes of groundwater were assumed. Its margin of exposure (MOE) would be more than 2,100,000, when calculated from its 'non-toxic level*' of $8.4 \, mg/kg/day$ and its estimated maximum exposure, and then divided by $10 \, due$ to the fact that 'non-toxic level*' was obtained from animal experiments. Since risk associated with exposure to this substance through food intakes from the environment is presumed to be minimal, this exposure will not increase MOE significantly, and no further action will be required at the moment to assess health risk from oral exposure to this substance.

As for its inhalation exposure, data at national-level were not available, and its health risk could not be assessed. Reports of its concentrations in the ambient air for some locations suggest that its maximum concentration at national level would be $0.075 \,\mu\text{g/m}^3$. For reference, when this is combined with its 'non-toxic level*' of $1.3 \,\text{mg/m}^3$ and then divided by 10 due to the fact that 'non-toxic level*' was obtained from animal experiments, MOE would be calculated to be 1,700. This substance is designated as a potential hazardous air pollutant. Domestic demand for it is relatively high, and it is exported relatively in large amounts. Its half-life in the atmosphere is $4.7 \,\text{to} \,47 \,\text{hrs}$. Almost all of its emission to the atmosphere is expected to remain there, so collection of information on its inhalation exposure would be required to assess health risk associated with its inhalation from the ambient air.

	Information of toxicity				Exposure assessment						
Exposure Path	Criteria for risk asse	essment	Animal	Criteria for diagnoses (endpoint)	Exposure medium	Predicted maximum exposure quantity and concentration		Result of risk assessment			Judgment
Oral	'Non-toxic level*, 8.4	mg/kg/day	Rats	Increase in relative	Drinking water	_	μg/kg/day	MOE	-	×	0
	ievei			liver weight	Groundwater	< 0.0004	μg/kg/day	MOE	> 2,100,000	0	
Inhalation	'Non-toxic	3	Rats	Atrophy/ hyperplasia of olfactory epithelia	Ambient air	_	μg/m³	MOE	_	×	(▲)
Innatation	level*,	1.3 mg/m ³			Indoor air		μg/m³	МОЕ	_	×	×

Non-toxic level *

- When a LOAEL is available, it is divided by 10 to obtain a level equivalent to NOAEL.
- When an adverse effect level is available for the short-term exposure, 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 48-h median effective concentration (EC₅₀) of 5,230 μ g/L for swimming inhibition in the crustacean *Daphnia magna*, and a 96-h median lethal concentration (LC₅₀) of 2,420 μ g/L for the fish species *Oryzias latipes* (medaka). Accordingly, based on these acute toxicity values and an assessment factor of 1,000, a predicted no effect concentration (PNEC) of 2.4 μ g/L was obtained.

With regard to chronic toxicity, reliable data of a 21-d no observed effect concentration (NOEC) of 1,000 μ g/L was obtained for reproductive inhibition in the crustacean *D. magna*. Accordingly, based on this chronic toxicity value and an assessment factor of 100, a predicted no effect concentration (PNEC) of 10 μ g/L was obtained. The value of 2.4 μ g/L obtained from the acute toxicity to the fish was used as the PNEC for this substance.

The PEC/PNEC ratio was less than 0.004 for both freshwater and seawater bodies. Accordingly, further work is thought to be unnecessary at this time.

Hazard assessment (basis for PNEC)				Predicted no	Exposure assessment				
Species	Acute/ chronic	Endpoint	Assessment factor	effect concentration PNEC (µg/L)	Water body	Predicted environmental concentration PEC (µg/L)	PEC/ PNEC ratio	Result of assessment	
Fish	Acuto	LC ₅₀	1 000	2.4	Freshwater	< 0.01	< 0.004	0	
(medaka)	Acute Mortality	Mortality	1,000	2.4	Seawater	< 0.01	< 0.004		

5. Conclusions

	Conclusions				
	Oral exposure No need for further work.		0		
Health risk	Inhalation and accomp	Risk unidentifiable. Collection of information considered	()		
	Inhalation exposure	necessary.	(\()		
Ecological risk	No need for further w	ork.	0		

[Risk judgments] O: No need for further work

▲: Requiring information collection

■: Candidates for further work

×: Impossibility of risk characterization

(O): Though a risk characterization cannot be determined, there would be little necessity of collecting information.

(lacktriangle): Further information collection would be required for risk characterization.