CAS No.: 104-51-8 Substance: *n*-Butylbenzene

Chemical Substances Control Law Reference No.: 3-11 (Butylbenzene), 3-21 (n-Alkylbenzene (C=3-36))

PRTR Law Cabinet Order No.:

Structural Formula:

Molecular Formula:  $C_{10}H_{14}$ Molecular Weight: 134.22

## 1. General information

The aqueous solubility of this substance is  $13.8 \text{ mg}/1000 \text{ g} (25^{\circ}\text{C})$ , the partition coefficient (1-octanol/water) (log  $K_{ow}$ ) is 4.26, and the vapor pressure is 1.13 mmHg (=150 Pa) (25°C). Its biodegradability (aerobic degradation) is characterized by a degradation rate of 72–80%. The substance does not have any hydrolyzable groups.

The main applications of this substance are as a synthetic intermediate and for liquid crystal manufacturing. The production (shipments) and import quantity in fiscal 2004 as n-alkyl benzene (C=3-36) were 100,000 to <1,000,000 t.

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## 2. Exposure assessment

Because this substance is not 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), 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.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, was estimated to be around 0.093  $\mu$ g/L for public freshwater bodies and less than around 0.01  $\mu$ g/L for seawater.

## 3. Initial assessment of ecological risk

With regard to acute toxicity, the following reliable data were obtained: a 72-h median effective concentration (EC<sub>50</sub>) of 15,90  $\mu$ g/L for growth inhibition in the green algae *Pseudokirchneriella subcapitata*; a 48-h EC<sub>50</sub> of 340  $\mu$ g/L for swimming inhibition in the crustacean *Daphnia magna*; and a 96-h median lethal concentration (LC<sub>50</sub>) of 3,330  $\mu$ g/L for the fish species *Oryzias latipes* (medaka). Accordingly, based on these acute toxicity values and an assessment factor of 100, a predicted no effect concentration (PNEC) of 3.4  $\mu$ g/L was obtained. With regard to chronic toxicity, the following reliable data were obtained: a 72-h no observed effect concentration (NOEC) of 424  $\mu$ g/L for growth inhibition in the green algae *P. subcapitata*; and a 21-d NOEC of 332  $\mu$ g/L for reproductive inhibition in the crustacean *D. magna*. Accordingly, based on these chronic toxicity values and an assessment factor of 100, a predicted no effect concentration (PNEC) of 3.3  $\mu$ g/L was obtained. The value of 3.3  $\mu$ g/L obtained from the chronic toxicity to the crustacean was used as the PNEC for this substance.

The PEC/PNEC ratio was 0.03 for freshwater bodies and less than 0.003 for seawater. 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)		Predicted environmental concentration PEC (µg/L)	PEC/ PNEC ratio	Result of assessment	
Crustacean	Chronic	NOEC Reproductive	100	3.3	Freshwater	0.093	0.03	0	
(water flea)	Cinome	inhibition	100	3.3	Seawater	< 0.01	< 0.003	O	

		Conclusions	
Ecological risk	No need for further work.		0
[Risk judgments	O: No need for further work	▲: Requiring information collection	
	■: Candidates for further work	×: Impossibility of risk characterization	
	(○) : Though a risk characterize	zation cannot be determined, there would be	little necessity
	collecting information.		
	( <b>A</b> ): Further information collect	ion would be required for risk characterization.	