9 CAS No.: 14938-35-3

Substance: 4-n-Pentylphenol

Chemical Substances Control Law Reference No.: 3-503 (as Monoalkyl (C =3-9) phenol)

PRTR Law Cabinet Order No.:

Structural Formula:

Molecular Formula: $C_{11}H_{16}O$ Molecular Weight: 164.24



1. General information

The aqueous solubility of this substance is 85 mg/L (25°C, calculated value), the partition coefficient (1-octanol/water) (log K_{ow}) is 4.06, and the vapor pressure is 0.011 mmHg (=1.5 Pa) (25°C, calculated value).

At this point in time, no information is available regarding the main applications of this substance, but the main applications of the branched alkyl group substance 4-*tert*-pentylphenol are believed to be a raw material for fine chemicals (dyestuff intermediates, rubber chemicals, surfactants, etc.) and a raw material for photographic materials. Production (shipments) and import quantity in fiscal 2004 as monoalkyl (C=3–9) phenol were 10,000 to <100,000 t.

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 proportion distributed to soil would be higher.

The predicted environmental concentration (PEC), which indicates exposure to aquatic organisms, was about 0.02 μ g/L for public freshwater bodies and less than about 0.01 μ 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_{50}) of 2,190 µg/L for growth inhibition in the green algae *Pseudokirchneriella subcapitata;* a 48-h EC_{50} of 899 µg/L for swimming inhibition in the crustacean *Daphnia magna;* a 96-h median lethal concentration (LC_{50}) of 1,250 µg/L for the fish species *Poecilia reticulata* (guppy); and a 96-h median lethal concentration (LC_{50}) of 3,710 µg/L for the great pond snail *Lymnaea stagnalis.* Accordingly, based on these acute toxicity values and an assessment factor of 100, a predicted no effect concentration (PNEC) of 9.0 µg/L was obtained. With regard to chronic toxicity, the following reliable data were obtained: a 72-h no observed effect concentration (NOEC) of 274 µg/L for growth inhibition in the green algae *P. subcapitata;* and a 21-d NOEC of 135 µg/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 1.4 µg/L obtained from the chronic toxicity to the crustacean was used as the PNEC for this substance.

The PEC/PNEC ratio was 0.01 for freshwater bodies and less than 0.007 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)	Water body	Predicted environmental concentration PEC (µg/L)	PE0 PNEC	C/ Result ratio assessm		of ent
	Crustacean (water flea)	Chronic	NOEC Reproductive inhibition	100	1.4	Freshwater	0.02	0.0	01	0	
						Seawater	< 0.01	<0.	007	0	
4.	. Conclusions										
		Conclusions							Judg	Judgment	
	Beological risk No need for further work.							0			
	Risk judgment	isk judgments] ○: No need for further work ▲: Requiring information collection									
Candidates for further work ×: Impossibility of risk characterization											
(\bigcirc) : Though a risk characterization cannot be determined, there would be little necessity of											
collecting information.											
(\blacktriangle) : Further information collection would be required for risk characterization.											