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| 16 | CAS No.: 618-85-9 | Substance: 3,5-Dinitrotoluene |
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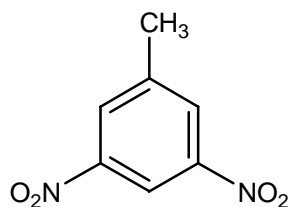
Chemical Substances Control Law Reference No.: 3-446 (as dinitrotoluene)

PRTR Law Cabinet Order No.: 1-157 (as dinitrotoluene)

Structural Formula:

Molecular Formula: C₇H₆N₂O₄

Molecular Weight: 182.14



1. General information

The aqueous solubility of this substance is 300 mg/L (25°C, calculated value) and the partition coefficient (1-octanol / water) (log Kow) is 2.2 (calculated value). The vapor pressure is 4.05×10^{-4} mmHg (= 5.40×10^{-2} Pa) (25°C, extrapolated value). Degradability (aerobic degradation) in terms of BOD-based degradation percentage is estimated to be 0%. The bioconcentration of this substance is thought to be zero or very low. In addition, this substance does not have hydrolyzable groups in the environment.

Dinitrotoluene is a Type 2 and Type 3 Monitoring Chemical Substance under the Law Concerning the Examination and Regulation of Manufacture, etc. of Chemical Substances and 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). It is used primarily as organic syntheses, a raw material of toluidine, dyes, and an intermediate compound of explosive. The quantity of production and import in FY2004 was 195 tons. The contents of Dinitrotoluene isomers in the general chemical products were approximately 75% for 2,4-Dinitrotoluene, approximately 20% for 2,6-Dinitrotoluene, and the content of 3,5-Dinitrotoluene is estimated to be less than 5%.

2. Exposure assessment

Total release of Dinitrotoluene to the environment in FY2004 under the PRTR Law came to approximately 0.68 tons, all of which was reported. Release to the public water bodies accounted for a large part of the reported release. Chemical Industry accounted for all of the reported release.

The distribution into each environment medium predicted by means of a multimedia model was 86.8% for water bodies and 10.0% for bottom in the case of the region where the release quantity to the environment and public water bodies was considered to be the maximum. In the case of the region where the release quantity to the atmosphere was considered to be the maximum, the distribution was 86.2% for water bodies and 9.9% for bottom.

No predicted maximum exposure concentration for inhalation exposure to human beings could be established. The predicted maximum oral exposure was estimated to be less than 0.02 µg/kg/day.

It was not possible to establish a predicted environmental concentration (PEC) that indicates exposure to aquatic organisms, as environmental concentrations sufficient for assessment have not been obtained.

3. Initial assessment of health risk

Dinitrotoluene (isomer mixture) may have effects on blood, and may produce methemoglobin. It may also lower consciousness and cause death at high concentration. The inhalation or ingestion may result in blue lips, nails and skin, drowsiness, nausea, vomiting, weakness, dizziness, headache, and laboured breathing. Contact with the skin may be absorbed and cause the similar symptoms.

Because the information of this substance about non-carcinogenic and carcinogenic effects is insufficient, the 'Non-toxicity level' and the carcinogenicity in humans cannot be determined. For inhalation, the exposure concentrations have not been

surveyed. Accordingly, its health risk cannot be identified.

The total release of Dinitrotoluene (DNT) to the environment (reported quantity of release) was 0.68 tons. Considering the fact that the content of this substance in DNT for industrial use is less than several percentages, and the identified of the health risks of 2,4-DNT and 2,6-DNT, there would be low necessity of collecting information of this substance for its health risk assessment.

| Information of toxicity | | | | Exposure assessment | | Result of risk assessment | | | Judgment |
|-------------------------|---------------------------------------|--------|-----------------------------------|---------------------|---|---------------------------|---|---|----------|
| Exposure path | Criteria for risk assessment | Animal | Criteria for diagnoses (endpoint) | Exposure medium | Predicted maximum exposure quantity and concentration | MOE | — | × | |
| Oral | 'Non toxic level' — mg/kg/day | — | — | Drinking water | — μg/kg/day | MOE | — | × | × |
| | | | | Groundwater | — μg/kg/day | MOE | — | × | |
| Inhalation | 'Non toxic level' — mg/m ³ | — | — | Ambient air | — μg/m ³ | MOE | — | × | × |
| | | | | Indoor air | — μg/m ³ | MOE | — | × | × |

4. Initial assessment of ecological risk

With regard to acute toxicity, reliable information of a 48-hour EC₅₀ immobilization value of 45,100 μg/L was found for the crustacea *Daphnia magna* (water flea), and a 96-hour LC₅₀ value of 22,600 μg/L was found for the fish *Pimephales promelas* (fathead minnow). Accordingly, an assessment factor of 1,000 was used, a predicted no effect concentration (PNEC) of 23 μg/L was obtained based on the acute toxicity values. As no information regarding chronic toxicity could be obtained, as the PNEC for the substance, a value of 23 μg/L was used.

At this point, the data about the environmental concentration of this substance have not been obtained, the assessment of the ecological risk could not be carried out. However, from the information about the percentage of contents of Dinitrotoluene isomers in general chemical products and PEC, it is considered that the further work on this substance may not be required.

| Hazard assessment (basis for PNEC) | | | Assessment factor | Predicted no effect concentration PNEC (μg/L) | Exposure assessment | | PEC/PNEC ratio | Result of assessment |
|------------------------------------|-----------------|----------------------------|-------------------|---|---------------------|--|----------------|----------------------|
| Species | Acute / chronic | Endpoint | | | Water body | Predicted environmental concentration PEC (μg/L) | | |
| Fish (fathead minnow) | Acute | LC ₅₀ Mortality | 1,000 | 23 | Freshwater | — | — | × |
| | | | | | Seawater | — | — | |

5. Conclusions

| | Conclusions | | Judgment |
|-----------------|--|---|----------|
| Health risk | Oral exposure | Impossible of risk characterization. However, there is thought to be comparatively little need to collect information, etc. | × |
| | Inhalation exposure | Impossible of risk characterization. However, there is thought to be comparatively little need to collect information, etc. | × |
| Ecological risk | Impossible of risk characterization. No need of further work at this time. | | × |

[Risk judgments] ○: No need of further work ▲: Requiring information collection
 ■: Candidates for further work ×: Impossible of risk characterization

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 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.