SIDS INITIAL ASSESSMENT PROFILE

CAS No.	111-82-0
Chemical Name	METHYL LAURATE
Structural Formula	

SUMMARY CONCLUSIONS OF THE SIAR

Physical-chemical properties

Methyl laurate is a colourless clear liquid. Measured melting point and boiling point are 5.2 °C and 267 °C respectively. Vapour pressure at 25 °C extrapolated from the experimental value is 0.161 Pa. Water solubility is < 4.40 mg/L at 20 °C or calculated to be 1.39 mg/L at 25 °C. Measured value of partition coefficient between octanol and water (log Kow) is 6.5 at 25 °C. Soil adsorption coefficient (log Koc) is calculated to be 3.11.

Human Health

No experimental information is available for toxicokinetics, metabolism, and distribution of methyl laurate. However, general information for medium-length linear esters indicates that they are rapidly absorbed from the gastrointestinal tract, hydrolyzed to yield the corresponding alcohols and carboxylic acids and further oxidized to carbon dioxide via the fatty acid pathway and excreted via the urine.

In an acute inhalation toxicity study (OECD TG 436), no deaths or signs of toxicity were observed at 5 mg/L in rats. Therefore, the aerosol inhalation LC_{50} value of methyl laurate was concluded to be over 5 mg/L. In acute oral toxicity studies (OECD TG 401), no deaths or signs of toxicity were observed at 20000 mg/kg bw in rats. Thus, the oral LD_{50} value of methyl laurate was concluded to be over 20000 mg/kg bw in rats.

Methyl laurate caused slight to severe skin irritation to rabbit skin, but reversibility was observed within 14 days after application (OECD TG 405). Methyl laurate caused no skin irritation in humans. *In vitro* skin irritation studies with human cultured cells showed no irritation. In the eye irritation tests in rabbits, no abnormality was found by application of methyl laurate. No information is available regarding the respiratory tract irritancy of methyl laurate.

Negative skin sensitization to methyl laurate was reported in a guinea pig maximization test (OECD TG 406).

In the combined oral repeated dose toxicity study with the reproduction/developmental toxicity screening test using rats (OECD TG 422) at doses of 0 (vehicle: corn oil), 250, 500 and 1000 mg/kg bw/d, methyl laurate did not cause any treatment-related effects at the highest dose tested. The NOAEL for oral repeated dose toxicity was considered to be 1000 mg/kg bw/d.

Methyl laurate did not induce gene mutation in *Salmonella typhimurium* TA98 TA100, TA1535, TA1537 and *Escherichia coli* WP2 *uvrA in vitro* tests (OECD TG 471 or 472). The substance did not induce chromosome aberrations in both cultured Chinese hamster lung (CHL/IU) cells and human lymphocytes (OECD TG 473). Based on these results, methyl laurate is considered to be non-genotoxic *in vitro*.

No data are available for the carcinogenicity of methyl laurate.

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In the combined oral repeated dose toxicity study with the reproduction/developmental toxicity screening test using rats (OECD TG 422), reproductive parameters and developmental parameters were not affected up to 1000 mg/kg bw/d. Based on these results, the NOAEL for reproductive and developmental toxicity was considered to be 1000 mg/kg bw/d.

Methyl laurate does not present a hazard for human health due to its low hazard profile. Adequate screening-level data are available to characterize the human health hazard for the purposes of the OECD Cooperative Chemicals Assessment Programme.

Environment

In the atmosphere, methyl laurate is expected to be degraded by hydroxyl radicals. A calculated half-life time of 0.811 days is obtained by AOPWIN (version 1.92a) for the indirect photo-oxidation by reaction with hydroxyl radicals in air.

In a study according to OECD test-guideline 111, methyl laurate was hydrolyzed at pH 9. Rate constant of 5.61×10^{-3} h⁻¹ and half-life time of 5.14 days were measured at 25 °C at pH 9. No experimental data are available at pH 4 and pH 7. According to HYDROWIN (ver. 2.00), a half-life time for this chemical at pH 7 is calculated to be 7.28 years.

An OECD test guideline 301C test was conducted with methyl laurate with activated sludge for four weeks. The concentration of the test substance was 100 mg/L and the concentration of the activated sludge was 30 mg/L as suspended solid matters. The test result showed 78 % degradation by BOD. BIOWIN (version 4.10) prediction shows that methyl laurate is readily biodegradable. According to these results, methyl laurate is considered to be readily biodegradable.

No information was available on the bioconcentration on methyl laurate. Using an octanol-water partition coefficient (log K_{ow}) of 6.5, a bioconcentration factor of 381 was calculated with BCFBAF (version 3.01). This chemical has a low potential for bioaccumulation.

Fugacity level III calculations show that methyl laurate is mainly distributed in soil (71.8 %) and water (19.9 %) compartments if equally and continuously released to the air, soil and water. A Henry's law constant of 302 Pa.m³/mole at 25 °C suggests that volatilization of methyl laurate from water is expected. A soil adsorption coefficient of log $K_{oc} = 3.11$ indicates methyl laurate has moderate potential for adsorption to soil and sediment.

The following acute toxicity test results have been determined for aquatic species:

Fish [Oryzias latipes]:	96 h $LC_{50} > 0.52$ mg/L (highest concentration, measured, flow-through), OECD-TG 203
Daphnid [Daphnia magna]:	48 h EC ₅₀ = 0.23 mg/L (measured, flow-through), OECD-TG 202
Algae [Pseudokirchneriella subcapitata]:	72 h ErC ₅₀ = 0.017 mg/L (measured, growth rate, static, closed), OECD-TG 201
	72 h EbC ₅₀ = 0.013 mg/L (measured, biomass*, static, closed), OECD-TG 201 * = area under growth curve
The following chronic toxicity test results have been determined for aquatic species:	
Daphnid [Daphnia magna]:	21 d LOEC = 0.21 mg/L (measured, flow-through), OECD-TG 211
	21 d NOEC = 0.081 mg/L (measured, flow-through), OECD-TG 211
Algae [Pseudokirchneriella subcapitata]:	72 h NOErC = 0.003 mg/L (measured, growth rate, static, closed), OECD-TG 201
	72 h NOEbC = 0.003 mg/L (measured, biomass, static, closed),

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OECD-TG 201

Methyl laurate possesses properties indicating a hazard for the environment (acute aquatic toxicity values between 0.01 and 1.0 mg/L for invertebrate and algae and chronic toxicity less than 0.1 mg/L for invertebrate and algae). However this chemical is considered to be readily biodegradable and has a low bioaccumulation potential. Adequate screening-level data are available to characterize the hazard to the environment for the purposes of the OECD Cooperative Chemicals Assessment Programme.

Exposure

Total amounts of production and import of methyl laurate in Japan (sponsor country) were reported to be 2,731 tonnes in the fiscal year 2010 according to the notification of annual manufactured and/or imported quantities of Priority Assessment Chemical Substances under Chemical Substances Control Law. In the United States, the total amount of production and/or import was reported to be 1 to 10 - 50 million pounds (4,540 to 22,680 tonnes) in 2006. Production volume in the world is not available.

Methyl laurate is manufactured by reaction of lauric acid with methanol in the presence of sulfuric acid. Methyl laurate is also produced as mixed fatty acid esters in Japan.

Methyl laurate is manufactured in closed system in Japan. Although small amounts of methyl laurate might be released into drains during cleaning of reaction vessels or packaging processes, the effluents are treated appropriately at sewage treatment facilities. As methyl laurate is readily biodegradable, release to the environment is small in Japan.

Methyl laurate is used as an industrial raw material such as an intermediate for emulsifiers, surface acting agents, or used as a paint additive in Japan. In the United States, methyl laurate is used as an intermediate according to Inventory Updated Reporting. Methyl laurate is also used as a food additive in Japan. In the Hazardous Substances Database, it is reported that methyl laurate is used as an intermediate for detergents, emulsifiers, wetting agents, stabilizers, lubricants, plasticizers, textiles, and flavouring agents. Methyl laurate is also used as a reference standard for gas chromatography and biochemical research. Methyl laurate is listed in the list of fragrance ingredients used in consumer goods published by the International Fragrance Association.

Occupational exposure through inhalation of vapour is anticipated when a worker handles this chemical directly. To prevent worker exposure to vapour, worker protection measures such as Local Exhaust ventilation or Personal Protective Equipment are necessary at production sites. Proper worker protection measures may be necessary at user sites as well.

As methyl laurate may be included in consumer products such as paints and fragrance or used as food additives, consumer exposure is anticipated. However, no detailed information was obtained for consumer exposure.

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