

21 November 2003

201-15058A

ROBUST SUMMARY FOR 1,5-CYCLOOCTADIENE

Summary

1,5-Cyclooctadiene is a colorless liquid with an aromatic odor and molecular weight of 108.20. It has a melting point of -70 to -69°C , a boiling point of 150.8°C at 757 mm Hg, specific gravity of 0.8818 at $25/4^{\circ}\text{C}$, and vapor pressure of 6.8 mm Hg at 25°C . 1,5-Cyclooctadiene is a flammable liquid with an autoignition temperature of 223°C and a flash point of 35°C . The octanol/water partitioning coefficient (log Kow) was determined to be 3.16. The bioconcentration factor (BCF) was estimated as 54.1, based on the empirical log Kow of 3.16; therefore, this compound has low potential to bioaccumulate. Since only an estimated water solubility value of 64.1 mg/L was available, a test following OECD guideline 105 is recommended.

A Henry's Law constant of 1.101×10^{-2} atm-m³/mole was estimated based on an estimated vapor pressure of 4.96 mm Hg and an estimated water solubility of 64.1 mg/L. The test substance is expected to have a half-life in air of 0.568 hours, with equal emissions to air, water, and soil. The estimated half-life in air as a result of reaction with OH radicals is estimated as 3.28 hours; for reactions with ozone the half-life is estimated as 41.256 minutes. Fugacity model predictions indicate that 1,5-cyclooctadiene will partition mainly to water and soil when emitted equally to air, water, and soil. Less than 2% will partition to air and sediments. Since the model for the environmental fate of 1,5-cyclooctadiene was run using estimated water solubility value, the model will be re-run using the newly acquired measured data. Although BIOWIN has estimated that primary biodegradation would occur in days to weeks and ultimate biodegradation would occur in weeks, a biodegradation study following OECD guideline 301 is recommended.

1,5-Cyclooctadiene was moderately toxic to aquatic fish and highly toxic to invertebrates with 48- and 96-hour LC₅₀s in rainbow trout of 30-38 mg/L, and a 24-hour LC₅₀ in *Daphnia* of 0.9 mg/L. The ECOSAR values (based on a measured log Kow of 3.16) for fish and *Daphnia* (6.5 mg/L and 7.6 mg/L, respectively) are consistent with the reported test data. Based on ECOSAR predictions, 1,5-cyclooctadiene would have a 96-hour EC₅₀ in green algae of 5.0 mg/L. ECOSAR predictions are generally substantiated by comparing the values obtained in the model to those obtained from actual testing of an analogous compound. Since no measured test data for an analogous chemical were available, and since ECOSAR predicts that algae are the most sensitive species, an algae study following OECD Guidelines 201 is recommended to determine toxicity to algae.

1,5-Cyclooctadiene had an oral LD₅₀ in rats of 2381 mg/kg. It was slightly toxic to rats via the inhalation route with a 4-hour ALC (approximate lethal concentration) of 2700 ppm and moderately toxic via the dermal route with a dermal LD₅₀ of > 3520 mg/kg. 1,5-Cyclooctadiene was a skin and eye irritant and a potent skin sensitizer. In a 2-week inhalation neurotoxicity study in rats at doses of 0, 50, 150, and 500 ppm, the NOEL (no-observed-effect level) was 150 ppm, based on decreased alerting response in rats during exposure and effects in the nose, kidneys, and urine of rats exposed to 500 ppm. No test substance-related findings in neuropathologic evaluation were observed at any level tested. No information regarding developmental or reproductive toxicity was available; therefore, a combined repeated dose

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toxicity study with the reproduction/developmental toxicity screening test via the oral route (OECD Guideline 422) is recommended.

1,5-Cyclooctadiene was negative for mutagenicity in *Salmonella typhimurium* and *E. coli*, negative for clastogenicity in human lymphocytes, and negative in an *in vivo* rat micronucleus assay.

Exposure Assessment for 1,5-Cyclooctadiene

1,5-Cyclooctadiene is manufactured at one DuPont facility. 1,5-Cyclooctadiene is a co-product produced in the manufacture of cyclododecatriene. 1,5-Cyclooctadiene is used as a chemical intermediate for the production of flame retardants, aroma chemicals, catalysts, and rubber goods.

The potential for exposure is the greatest during the loading and unloading of 1,5-cyclooctadiene since closed processes are used on the site. The site can have approximately 1100 personnel working (construction, contractor, and plant employees). The areas where the substance is manufactured will have 16 total operators during normal operations and 40 people during a shutdown or major construction activity.

The site has effective safety, health, and environmental practices and procedures in addition to engineering controls, environmental controls, and personal protective equipment to control exposure. Adequate safety equipment, such as safety showers, eyewash fountains, and washing facilities, are available in the event of an occupational exposure. Individuals handling 1,5-cyclooctadiene should wear safety glasses and impervious clothing, such as gloves, apron, boots, or whole bodysuit made of nitrile rubber or Viton. When the possibility exists for eye and face contact due to splashing or spraying of material, chemical splash goggles and face shield should be worn. DuPont practices responsible care and assesses the ability of potential customers to safely handle 1,5-cyclooctadiene prior to commencing a commercial relationship. The Product Stewardship System works with customers to understand their applications and any issues associated with PPE (personal protective equipment), safety equipment (safety showers, eyewash stations, ventilation needs, etc.), storage concerns, disposal requirements, and MSDS questions.

Air monitoring has been conducted on 1,5-cyclooctadiene using the site Industrial Hygiene Procedure (OSHA 07). LOGAN (lognormal analysis) is a computerized statistical method for characterizing occupational exposures to chemicals, noise, and other environmental hazards. LOGAN uses sequential collection of data and makes decisions on the minimum amount of data. It helps make cost-effective, accurate decisions that ensure a healthy workplace. LOGAN uses inferential statistics to estimate the true workplace conditions, in the same way that public polling estimates opinions by sampling a representative percentage of the public. LOGAN is designed to limit the risk of employee occupational overexposure to less than 5%.

The DuPont Acceptable Exposure Limit for 1,5-cyclooctadiene is 10 ppm, 8- and 12-hour TWA. No other limits have been established. None of the samples taken suggest the probability of exposure in excess of the current recommended AEL of 10 ppm, 8- and 12-hour TWA.

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EXPOSURE DATA

Area: Operators and Maintenance

| | People | No. of Results | Avg. of TWA (ppm) | Min. of Results (ppm) | Max. of TWA (ppm) |
|-------------|-----------------|----------------|-------------------|-----------------------|-------------------|
| Production | 16 (since 1990) | 403 | 0.07 | <0.01 | 2.47 |
| Maintenance | 30 (since 1990) | 153 | 0.13 | <0.01 | 0.13 |

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TEST PLAN FOR 1,5-CYCLOOCTADIENE

| 1,5-Cyclooctadiene CAS No. 111-78-4 | Data Available | Data Acceptable | Testing Required |
|--|-----------------------|------------------------|-------------------------|
| | Y/N | Y/N | Y/N |
| PHYSICAL/CHEMICAL CHARACTERISTICS | | | |
| Melting Point | Y | Y | N |
| Boiling Point | Y | Y | N |
| Vapor Pressure | Y | Y | N |
| Partition Coefficient | Y | Y | N |
| Water Solubility | Y | N | Y |
| ENVIRONMENTAL FATE | | | |
| Photodegradation | Y | Y | N |
| Stability in Water | Y | Y | N |
| Transport (Fugacity) | Y | N | Y* |
| Biodegradation | Y | N | Y |
| ECOTOXICITY | | | |
| Acute Toxicity to Fish | Y | Y | N |
| Acute Toxicity to Invertebrates | Y | Y | N |
| Acute Toxicity to Aquatic Plants | N | N | Y |
| MAMMALIAN TOXICITY | | | |
| Acute Toxicity | Y | Y | N |
| Repeated Dose Toxicity | Y | N | Y |
| Developmental Toxicity | N | N | Y |
| Reproductive Toxicity | N | N | Y |
| Genetic Toxicity Bacterial Gene Mutations | Y | Y | N |
| Genetic Toxicity <i>in vitro</i> Chromosomal Aberrations | Y | Y | N |
| Genetic Toxicity <i>in vivo</i> Micronucleus | Y | Y | N |
| * After testing is complete for water solubility, fugacity model will be run using measured water solubility data. | | | |