

**ROBUST SUMMARIES FOR**  
**Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester**

**1.0 GENERAL INFORMATION**

**1.1 CAS NUMBER** 61898-95-1  
**1.2 CHEMICAL NAME** Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester

**2.0 PHYSICAL AND CHEMICAL DATA**

**2.1 MELTING POINT**

**Test Substance:** Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester  
**Remarks:** The material is a liquid at room temperature. See Boiling Point.

**2.2 BOILING POINT**

**Test Substance:** Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester  
**Method:** Distillation  
**GLP:** No  
**Year:** 1981  
**Results:** 78 °C at 0.6 mm Hg  
**Data Quality:** 4b  
**References:** FMC Chemical Data Sheet No. 174, Revision 1, 1981

**2.3 VAPOR PRESSURE**

**Test Substance:** Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester  
**Method:** Gas saturation technique, mathematical extrapolation from higher temperature data.  
**GLP:** No  
**Year:** 1981  
**Results:** 0.03 mm Hg at 25 °C  
**Data Quality:** 4b  
**References:** FMC Chemical Data Sheet No. 174, Revision 1, 1981

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## 2.4 PARTITION COEFFICIENT

Test Substance: Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester  
Method: OPPTS 830.7550  
Temperature: 20 °C  
GLP: Yes  
Year: 2003  
Results: 4600 (logK<sub>ow</sub> = 3.66)  
Shake Flask Method  
Data Quality: 1a  
References: ABC Laboratories, Inc., Columbia Missouri

## 2.5 WATER SOLUBILITY

Test Substance: Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester  
Method: Shake flask/gas chromatography  
Temperature: 25 °C  
GLP: No  
Year: 1998  
Results: 53 µg/mL  
Data Quality: 4b  
References: FMC Memorandum, M. Alvarez to W. W. Smith, 6/16/98

## 3.0 ENVIRONMENTAL FATE AND PATHWAY

### 3.1 PHOTODEGRADATION

Test Substance: Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester  
Method: Estimated by the AOP program (v. 1.90) which estimates rate constants and half-lives of atmospheric reactions of organic compounds with hydroxyl radicals and ozone in the atmosphere.  
GLP: No  
Year: 2000

Results: For reaction with hydroxyl radicals, the predicted half-life is 2.4 days with a rate constant of  $4.46 \times 10^{-12}$  cm<sup>3</sup>/molecule-sec.

Remarks: The photodegradation calculation by an acceptable method is assigned a reliability code of 2f.

References: AOPWIN version 1.90, Syracuse Research Corporation, Syracuse, NY

### 3.2 STABILITY IN WATER (HYDROLYSIS)

Test Substance: Cyclopropanecarboxylic acid, 3-(2,2-dichloroethyl)-2,2-dimethyl-, methyl ester

Method: Estimated by HYDROWIN program (v. 1.67)

GLP: No

Year: 2000

Results: This compound was predicted to undergo base hydrolysis.

Rate constant (pH>8, 25 °C): 1.27E-2 L/mol-sec

Half-life at pH 8: 1.7 years

Half-life at pH 7: 17 years

Remarks: The hydrolysis calculation by an acceptable method is assigned a reliability code of 2f.

References: HYDROWIN version 1.67, Syracuse Research Corporation, Syracuse, NY

### 3.3 TRANSPORT/DISTRIBUTION (FUGACITY MODEL)

Test Substance: Cyclopropanecarboxylic acid, 3-(2,2-dichloroethyl)-2,2-dimethyl-, methyl ester

Method: Estimated by EPIWIN program (v. 3.11) Level III Fugacity Model

Input parameters from user: chemical structure (SMILES notation): COC(=O)C1C(C=C(Cl)Cl)C1(C)C

Log Kow: 3.66

Water solubility: 53 mg/L

Vapor pressure: 0.03 mm Hg

Boiling point: 78 °C

Input calculated by the model: Henry's law constant: 1.6E-04 atm m<sup>3</sup>/mol

Koc: 285.7

Half-life in Air: 54.9 hr

Half-life in Water: 900 hr

	Half-life in Soil	900 hr
	Half-life in Sediment	3600 hr
GLP:	No	
Year:	2004	
Results:	Distribution using Level III Fugacity Model	
	Air	3.53%
	Water	21.4%
	Soil	73.7%
	Sediment	1.42%

Remarks: Code 2f

References: EPIWIN version 3.11, U.S. Environmental Protection Agency and Syracuse Research Corporation, Syracuse, NY

**Description of EPI-WIN Fugacity Model (Help File Excerpt):**

EPIWIN v3 contains a Level III fugacity model. The methodology and programming approach was developed by Dr. Donald Mackay and co-workers (Mackay et al., 1996a, 1996b; Mackay 1991). The model in EPIWIN v3 is a direct adaptation of this methodology and approach. While it uses the same equations as Mackay's EQC Level III Fugacity Model, it was adapted specifically for use in EPIWIN. It uses exactly the same default values as the Mackay model (Note: an executable version of Mackay's EQC model can be downloaded from The Environmental Modeling Centre (Trent University) Internet web-site: <http://www.trentu.ca/academic/aminss/envmodel/models.html>).

A detailed description of Level I, II and III fugacity models is not presented here; please see the Mackay publications and Internet web-site cited above. In general, fugacity models predict the partitioning of an organic compound in an evaluative environment. A Level III model does not assume an equilibrium state; it only assumes steady-state. The Level III model in EPI predicts partitioning between air, soil, sediment and water using various user-input parameters and/or inputs estimated by several EPI programs.

Note: all Fugacity Half-Life Values, Emission Values, Soil Koc and Advection Values have default values or estimation methods. User intervention is not required to generate model predictions. However, more accurate user-input data (e.g. measured half-live data) should result in better model predictions. Also, modification of various default values may be required for individual evaluations. A discussion of each "Fugacity" menu selection follows.

**Half-Life Values**

Half-lives are required for air, soil, sediment and water ... the fugacity cannot run without them.

If the half-lives in air, water, soil and sediment are known, the "Use Half-Lives Entered Below" should be selected and the known values should be entered in the appropriate fields. Often, however, this data is not available and requires estimation. The BIOWIN and AOPWIN programs are used to make these estimates. The AOPWIN air estimate is based upon estimated hydroxyl radical and ozone rate constants. AOPWIN does have an experimental database containing more than 700 compounds. If an entered structure has a database match, the database value is used instead of the program estimate.

The water, soil and sediment half-lives are based upon BOWIN prediction times for either ultimate or primary biodegradation. The prediction times range from “Hours” to “Recalcitrant”. Each “time-range” has a default half-life value; these default values can be changed if desired. The default values were derived by Dr. Robert S. Boethling of the U.S. EPA based upon the methodology reported in the Boethling et al. (1994) journal article. The default values in EPI v3.02+ are slightly different than the default values in prior versions of EPI. If BOWIN predicts “Weeks” for biodegradation, then a half-life of 15 days is applied to water and soil ... a half-life of 60 days is applied to sediment because the default “Half-Life Factor” for sediment is 4 times the value for water and soil (again, the default “Half-Life Factors” were derived by Dr. Robert S. Boethling). Each Biowin half-life is multiplied by the “Half-Life Factors”.

The Half-life entry box contains two buttons for “Set Biowin Half-life Values”. The “EPA default” button sets the values derived by Dr. Robert S. Boethling. The “Alternative” button sets slightly more conservative values.

#### **Emission Values**

The default Environmental Emission Rates are 1000 kg/hr to Air, Water and Soil (Sediment has a value of zero); these are the Mackay defaults. The Air, Water and Soil rates can be modified if desired.

EPIWIN can run the level III model once per EPI run using the emission rates shown (this is the program default) or multiple times per EPI run. Currently, “Multiple Level III Output” will run the Level III model 7 times using all permutations of Air, Water and Soil rates as either 0 or 1000 (the permutation where all rates are 0 is excluded).

#### **Advection Values**

The Advection Times apply to Air, Water and Sediment. These values should not be changed unless you are very familiar with the Mackay model. Access is available for advanced use only.

#### **Soil Koc Value**

The Fugacity Model requires a soil Koc value. By default, the Mackay Model calculates the soil Koc from the log Kow value. If desired, the soil Koc can be estimated by the PCKOCWIN program or directly entered by the user.

#### **Other Input Parameters**

The Fugacity Model cannot run without a vapor pressure. If the vapor pressure is not user-entered, the model uses the vapor pressure estimate by the MPBPWIN Program. If the MPBPWIN Program estimates a vapor pressure of zero (which can occur if an estimate is less than 1.00e-40 mm Hg), the fugacity model uses an assumed value of 1.00e-15 mm Hg (this value is low enough to have no sensitivity effect in the fugacity estimates). See section 5.3 concerning Henry’s law constant inputs. The model also requires a log Kow value. If the log Kow is not user-entered, the model uses the value from the KOWWIN Program (an experimental database value is used if available instead of the estimate).

The Fugacity model in EPIWIN has limited user-access to many parameters in the Mackay Level III Model. For example, parameters such as rain rate, aerosol deposition, soil water runoff, and diffusion mass transfer coefficients cannot be changed by the EPIWIN user. For these parameters, EPIWIN relies solely upon the defaults values as determined by Mackay and co-workers. This greatly simplifies application of a Level III model for most users. If you understand the inter-workings of a Level III model and need access to these parameters, you can download the Mackay EQC Model from the Internet web-site listed above.

### **3.4 BIODEGRADATION**

Test Substance: [Cyclopropanecarboxylic acid, 3-\(2,2-dichloroethenyl\)-2,2-dimethyl-, methyl ester](#)

Method: [OECD guideline 301D, OPPTS 835.3110](#)

Test type: Closed bottle test

Contact time: 28 days

Inoculum: secondary clarifier supernatant from a wastewater treatment plant

Test conditions: Aerated mineral medium was dosed with 2 mg/L of methallyl chloride and approximately 0.5 mL of inoculum. Samples were kept at 21-22 °C and sampled 0, 7, 14, 21 and 28 days after treatment. The test contained an inoculum control group, a phthalic acid reference group and a treatment group. Degradation was followed by the analysis of dissolved oxygen. The dissolved oxygen uptake of the test solution (corrected for uptake of blank inoculum) was expressed as a percentage of the theoretical oxygen demand of the test substance.

GLP: yes

Year: 2003

Results: The percent degradation after 28 days was 0%.

References: Schaefer, E.C. and Siddiqui, A.I., "Methyl DV Ester: An Evaluation of Ready Biodegradability Using the Closed Bottle Test Method", Unpublished study for FMC Corporation, Agricultural Products Group, Princeton, NJ, Report PC-0322, May 2004.

#### 4.0 ECOTOXICOLOGY

##### 4.1 ACUTE TOXICITY TO FISH

Test Substance: Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester (99.3%)

Method: U.S. EPA FIFRA 72-1 (c)

The acute toxicity under static renewal conditions of cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester to the rainbow trout (*Oncorhynchus mykiss*), was conducted for FMC Corporation for 96-hours from May 24 to 28, 1999 at T.R. Wilbury Laboratories, Inc., in Marblehead, Massachusetts.

The test was performed at 12 +/- 1°C with five concentrations of test substance and a dilution water control. The dilution water was deionized water collected at Marblehead, MA and adjusted to a hardness of 40 to 48 mg/L as CaCO<sub>3</sub>. Dissolved oxygen, pH, conductivity, temperature were measured and recorded daily in each test chamber that contained live animals. Measurements were made before and after media renewal at 24, 48, and 72 hours.

Juvenile rainbow trout were obtained from a single source and were identified using an appropriate taxonomic key. They were obtained from a commercial supplier on May 6, 1999. Prior to testing fish were maintained under flow-through conditions and were fed a commercial flake food daily during acclimation except for the 48 hours immediately preceding the test initiation. Fish were not fed during the test. Nominal concentrations were 0, 3.9, 6.5, 11, 18, and 30 mg/L based on a range-finding test. The first definitive test was attempted under daily renewal conditions but was repeated after poor analytical recoveries of the test material. The second definitive test was also repeated because of poor recoveries. The final definitive toxicity test was conducted for 96 hours from May 24 to

28, 1999. Nominal concentrations were 2.6, 4.3, 7.2, 12, and 20 mg/L. It was performed under static renewal conditions and fish were transferred daily to vessels containing freshly prepared solutions.

Ten rainbow trout were indiscriminately distributed to each of two replicates of each treatment. The test was performed in 3.8-liter glass jars that contained 3.0 liters of test solution. Test vessels were randomly arranged in a water bath during the test. A 16-hour light and 8-hour dark photoperiod was automatically maintained with cool-white fluorescent lights that provided a light intensity of approximately 80 foot-candles. The number of surviving organisms, the occurrence of sub lethal effects, and observations of insolubility were determined visually and recorded initially and after 24, 48, 72, and 96 hours. Dead organisms were removed every 24 hours or when first observed.

Results of the toxicity test were interpreted by standard statistical techniques. The 24 hour LC50 was calculated by the binomial method and the 48, 72, and 96 hour LC50 values and slope of the concentration-response curve were determined using the probit method. The no observed effect concentration (NOEC) is the highest concentration of test substance that allowed at least 95% survival and did not cause any sub lethal effects.

Species:	Rainbow Trout ( <i>Oncorhynchus mykiss</i> )
Test Concentration:	0 (control), 2.56, 4.09, 6.44, 10.7, and 18.5 mg/L (measured)
Exposure Period:	96 hours
Analytical Monitoring:	Analytical determination of test substance concentration was performed from each concentration at the beginning and end of the test. Samples were analyzed using a gas chromatograph equipped with an electron capture detector and an HP Chem DOS data system.
GLP:	Yes
Year:	1999
Results:	<p>Insoluble material was not observed at any time during the test. Mean measured concentrations of cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester were ND (none detected at or above the quantitation of 0.354 mg/L; control), 2.56, 4.09, 6.44, 10.7, and 18.5 mg/L. Mean measured concentrations were 89 to 98% of nominal values, and were stable during the 96-hour test.</p> <p>Ninety-five percent survival occurred in the control and no sub lethal effects were noted in the control at the end of the exposure period. During the definitive toxicity test the conductivity range was 150 to 180 umhos/cm (mean = 160 umhos/cm), the pH ranged from 7.0 to 7.9, the temperature ranged for 12.0 to 12.9 °C (mean = 12.6 °C), and the dissolved oxygen concentration ranged from 5.9 to 9.8 mg/L (mean = 8.5 mg/L).</p> <p>Exposure of rainbow trout to the test substance resulted in a 96-hour LC50 of 3.01 mg/L (95% confidence interval = 2.63 to 3.39 mg/L) and a 96-hour NOEC of less than 2.56 mg/L. The slope of the 96-hour dose response curve is 9.7.</p>
Data Quality:	1a

References: Acute Toxicity of DV Methyl Ester to the Rainbow Trout, *Oncorhynchus mykiss*). T.R. Wilbury Laboratories, Inc.; Study Number 1580-FM, FMC Study Number A98-4810

#### 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Test Substance: Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester (99.3%)

Method: U.S. EPA FIFRA 72-2

The acute toxicity under static renewal conditions of cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester to the daphnid, *Daphnia magna*, was conducted for FMC Corporation for 48 hours from February 15 to 17, 1999 at T.R. Wilbury Laboratories, Inc., in Marblehead, Massachusetts.

The test was performed at 20 +/- 1°C with five concentrations of test substance and a dilution water control. The dilution water was deionized water collected at Marblehead, MA and adjusted to a hardness of 160 to 180 mg/L as CaCO<sub>3</sub>. The pH of the dilution water was adjusted to less than 8.0 prior to use. The dissolved oxygen concentration was always at least 7.6 mg/L.

Juvenile daphnids used in the test were obtained from an in-house culture that was acclimated to test conditions for more than seven days at T.R. Wilbury Laboratories. During the acclimation period, the daphnia culture was supplied yeast/trout chow suspension and *Selenastrum capricornutum* daily. Daphnids were not fed during the test. Based on range-finding tests, nominal concentrations tested were 0mg/L (control) 3.9, 6.6, 11, 18 and 30 mg/L. The loading rate during the test was approximately 14 mg/L and it was less than or equal to 40 daphnids per liter. All animals were in good condition at the beginning of the study.

Ten daphnids were indiscriminately distributed to each of two replicates of each treatment concentration. The test was performed in 300 mL glass beakers that contained 250 mL of test solution. Test vessels were randomly arranged in a water bath for the 48-hour test. A 16-hour light and 8-hour dark photoperiod was automatically maintained at approximately 50 footcandles. Aeration was not required to maintain dissolved oxygen above acceptable limits. The number of surviving organisms, the occurrence of sub-lethal effects, and observations of insolubility were determined visually and recorded initially and after 24 and 48 hours. Dead organisms were removed every 24 hours or when first observed.

Statistical methods were used to determine the 24 and 48-hour LC50 values and 24 and 48-hour EC50 values. Calculations were performed using the binomial or probit method and mean measured concentrations of test substance.

Species: Daphnid, *Daphnia magna*

Test Concentration: 0 (control), 3.04, 5.13, 9.01, 14.6 and 23.6 mg/L(measured)

Exposure Period: 48 hours

Analytical Monitoring: Analytical determination of test substance concentration was performed from each concentration at the beginning and end of the test. Samples were analyzed using a gas chromatograph equipped with an electron capture detector and an HP Chem DOS data system. Aliquots were extracted, partitioned and concentrated prior to being analyzed.

GLP: Yes

Year: 1999

Results: After 48 hours of exposure the control organisms had an average wet weight (blotted dry) of 0.34 mg. Insoluble material was not observed at any time during the test. Mean measured concentrations of cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester were ND (none detected at or above the quantitation of 0.373 mg/L; control), 3.04, 5.13, 9.01, 14.6 and 23.6 mg/L. Mean measured concentration were 78 to 82% of nominal values.

One hundred percent survival occurred in the control and no sub-lethal effects were noted in the control during the exposure period. The conductivity ranged from 600 to 610 umhos/cm, the pH ranged from 7.4 to 7.6, the temperature ranged from 20.2 to 21.1°C, and the dissolved oxygen concentration ranged from 8.5 to 8.9 mg/L.

Exposure to daphnids with cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester resulted in a 48-hour median lethal concentration (LC50) of 7.04 mg/L (95% confidence interval = 6.03 to 8.19 mg/L) and a 48-hour median effective concentration (EC50) of 6.40 mg/L (95% confidence interval = 5.13 to 9.01 mg/L). The 48-hour NOEC is 3.04 mg/L. At 9.01 mg/L test concentration, organisms experienced immobilization at the 24 and 48 hour observations.

Data Quality: 1a

References: Acute Toxicity of DV Methyl Ester to the Daphnid, *Daphnia magna*. T.R. Wilbury Laboratories, Inc.; Study Number 1581-FM, FMC Study Number A98-4809

### 4.3 TOXICITY TO AQUATIC PLANTS

Test Substance: Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester (99.3%)

Method: U.S. EPA FIFRA Subdivision J, 123-2

The toxicity of cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester to the freshwater algae, *Selenastrum capricornutum*, was conducted for FMC Corporation for 120 hours from February 3 to 8, 1999 at T.R. Wilbury Laboratories, Inc., in Marblehead, Massachusetts.

The test was conducted under static conditions at 24 +/- 2°C with five concentrations of test substance and a dilution water control. The dilution water was sterile enriched medium adjusted to pH of 7.5 +/- 0.1. The number of cells/mL was determined microscopically using a haemocytometer every 24 hours during the exposure. Based on range-finding tests, nominal concentrations used were 0 mg/L (control), 2.0, 4.0, 7.9, 16, and 32 mg/L.

Algae used in the test were obtained from a culture procured from the Culture Collection of Algae at the University of Texas at Austin and delivered to T.R. Wilbury Laboratories, Inc. The culture was transferred to sterile enriched media identical to media used for the test and maintained at test conditions for more than 14 days before the definitive test. The sub-sample of algae used to inoculate media at the start of the test came from a five day old culture.

Algae were distributed among four replicates of each treatment at approximately 3,000 cells/mL.

The fourth replicate was established to allow the measurement of pH at 72 hours. Test vessels were 250 mL glass flasks that contained 50 mL of test solution. Vessels were capped with inverted glass beakers and randomly arranged on a rotary shaker that was adjusted to 100 rpm and located in an incubator during the test. A 24-hour light and 0-hour dark photoperiod was automatically maintained with a light intensity of 4,300 to 4,400 lux.

The number of algal cells/mL in each test vessel and the occurrence of relative size differences, unusual cell shapes, colors, flocculations, adherence of cells to test containers, or aggregation of cells was determined microscopically using a haemocytometer. Temperature of the incubator was measured and recorded daily, and pH was determined in each test vessel at the beginning and end of the test. The pH of each fourth replicate was determined at 72 hours. The temperature of a representative flask of water incubated among the test vessels was recorded continuously.

Results of the toxicity test were interpreted by standard statistical methods. The average specific growth rate was calculated as the natural log of the number of cells/mL at 24, 48, 72, 96 and 120 hours of exposure, minus the natural log of the number of cells/mL at 0 hours of exposure, divided by the hours of exposure. All statistical analyses were performed using the number of cells/mL and the average growth rate, both with the measured concentrations of test substance.

Species:	<i>Selenastrum capricornutum</i>
Test Concentration:	<0.373 mg/L; (control), 2.00, 3.76, 7.63, 15.9 and 31.1 measured
Exposure Period:	120 hours
Analytical Monitoring:	Analytical determination of test substance concentration was performed from each concentration at the beginning and end of the test. Samples were analyzed using a gas chromatograph equipped with an electron capture detector and an HP Chem DOS data system. Aliquots were extracted, partitioned and concentrated prior to being analyzed.
GLP:	Yes
Year:	1999
Results:	<p>The 24-hour EC25 and EC50 could not be calculated because growth at all tested concentrations and the control was less than 10,000 cells/mL. The 48, 72, 96 and 120-hour effective concentrations were calculated using the weighted least squares non-linear regression estimation procedure. The 120-hour no observed effect concentration for algae growth was also calculated. A Chi<sup>2</sup> test was used to determine that data were normally distributed and Bartlett's test was used to determine that variances were homogeneous. Based on these results, a one-way analysis of variance and Dunnett's test were used to compare treatment and control data.</p> <p>Insoluble material was not observed at any time during the test. Initial measured concentrations of cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester were &lt;0.373 mg/L (control), 2.00, 3.76, 7.63, 15.9 and 31.1 mg/L. Initial measured concentrations were 94 to 100% of nominal values but final concentrations averaged 5.5 to 29%. For this reason, initial measured concentrations were used for all calculations. The algal population in the control vessels grew well, increasing from an average of 3,000 cells/mL to an average of</p>

5,927,000 cells/mL after 120 hours of exposure. Water quality throughout the test was within acceptable limits. The range of the incubator temperatures was 23.5 to 23.7°C and the pH of test media was not significantly affected by the test substance at the beginning of the test.

Exposure of *Selenastrum capricornutum* to cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester for 96 hours resulted in a median effective concentration (EC50) of 5.22 mg/L when using the number of cells/mL and 8.26 mg/L when calculated using the average specific growth rate. Exposure of *Selenastrum capricornutum* for 120 hours resulted in a median effective concentration (EC50) of 8.03 mg/L when using the number of cells/mL and 8.69 mg/L when calculated using the average specific growth rate. The 120-hour NOEC is 3.76 mg/L when calculated using either the number of cells/mL or the average specific growth rate.

Data Quality:

1a

References:

Growth and Reproduction Toxicity Test with DV Methyl Ester and the Freshwater Alga, *Selenastrum capricornutum*. T.R. Wilbury Laboratories, Inc.; Study Number 1582-FM, FMC Study Number A98-4808

## 5.0 TOXICITY

### 5.1 ACUTE TOXICITY

#### 5.1.1 ORAL

Test Substance:

Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester (>98%)

Method:

US EPA, 1982, Subdivision F, Hazard Evaluation, 81-1

An acute oral LD50 study was conducted with test material administered undiluted by gavage. Young adult Sprague-Dawley rats were received from Taconic Farms, Germantown, New York. The rats were randomized into their cages using a computer-generated table of random numbers. The animals were acclimated for a minimum of seven days. The condition of the animals was examined prior to formally being released for the study. Fresh tap water and Purina Laboratory Rat Cow 5001 were provided *ad libitum*. Room temperature is to be maintained from 70°F +/- 10°F during the study, and relative humidity will be monitored daily. The animals were individually housed in stainless steel suspended rat cages and maintained in a room with a 12-hour fluorescent light and 12-hour dark cycle.

Animals were fasted overnight prior to dosing. Immediately prior to dosing, male body weights ranged from 217 to 236 grams and female weights were between 201 and 230 grams. The 5000 mg/kg dose of test material was administered as a single treatment via gavage directly into the stomach of each animal approximately four hours after initiation of the light cycle. Observations for mortality and clinical signs were conducted at 0.5, 1, 2, 3, 4 and 6 hours on the day of dosing and twice daily for 13 days. On day 14 the animals were observed once. Body weights were recorded on days 0, 7 and 14 of study. Animals dying intercurrently were weighed upon discovery of death. Gross necropsies were performed on all animals that died during the study. Survivors were euthanized with CO2 gas on day 14 and submitted to gross necropsy.

Species/strain:

Sprague-Dawley rats

Sex: Males and females

No. Animals/Group: 5/sex/group

Post dosing observation period: 14 days

GLP: Yes

Year: 1985

Results: Room temperature was maintained from 70°F to 78°F during the study, while relative humidity ranged from 42% to 57%. Predominant clinical signs included abdominogenital staining, ataxia, chromodacryorrhea, chromorhinorrhea, cyanosis, diarrhea, exophthalmos, lacrimation, decreased locomotion, oral discharge, prostration and recumbency. One female rat died within three days of dosing. All surviving rats returned to normal by the 5<sup>th</sup> day of the study. All surviving animals gained weight during the study. At necropsy, one rat had a mass located in the anogenital area between the skin and muscle layers gross

The test material is classified as practically non-toxic to adult rats under the conditions of this study. The oral LD50 is greater than 5,000 mg/kg in both male and female rats.

Data Quality: 1a

References: Acute Oral Toxicity of FMC 39338 in Rats, FMC Toxicology Laboratory, FMC Study Number A84-1410

### 5.1.2 INHALATION

Test Substance: Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester (>98%)

Method: No guideline mentioned.

Young adult Sprague-Dawley rats were received from Taconic Farms, Germantown, New York. The animals were randomized into their cages using a computer-generated table of random numbers. The condition of the animals was examined prior to being formally released for the study. Fresh tap water and Purina Laboratory Chow 5001 were available *ad libitum*, except during exposure. The animals were individually housed in stainless steel suspended rat cages and maintained in a room with a 12-hour fluorescent light and 12-hour dark cycle.

Two groups (exposure and control) of five male and five female rats each were used for this study. Male body weights ranged from 262 grams to 302 grams and female body weights ranged from 232 grams to 261 grams immediately prior to exposure. The test chamber was made of stainless steel and glass and had a volume of 100 liters. The chamber air was exhausted from the bottom of the chamber and passed through a commercial airline filter, containing particulate and organic vapor cartridges. The exhaust was powered by a laboratory vacuum pump at a flow rate of 20 liters per minute, creating a slightly negative pressure in the chamber, which was considered to be the total chamber airflow rate. The entire exposure system and exhaust filter were contained in a fume hood. The calculated 99% equilibrium time for the chamber at a flow rate of 20L/min was 23 minutes (equivalent to 12 air changes per hour). The test animals were randomly assigned to and housed in individual compartments of a wire mesh cage bank (all on the same horizontal level) of the test chamber.

The rats were exposed to saturated vapors of cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester for six hours at a nominal concentration of 38.7 ppm in a dynamically operated, whole-body inhalation exposure chamber. Chamber air samples were taken continuously with a Bendix THC analyzer, calibrated for methane, during the exposure. Readings each 30 minutes were used to determine the airborne concentration of test material. At the end of exposure, the chamber was cleared for 31 minutes by drawing room air through it at the same flow rate as the test material prior to removing the animals from the chamber. The control group was sham-exposed using room air only and the same basic exposure system. Chamber air temperature and relative humidity were monitored continuously during the exposure with wet/dry bulb hygrometers mounted inside the chambers at 30-minute intervals.

Observations for toxicity and mortality were performed every fifteen minutes during the first hour of exposure, hourly for the remainder of exposure, upon removal from the chamber, at seven hours post-exposure, twice daily thereafter for thirteen days and once on day 14. Individual body weights were recorded immediately prior to exposure (day 0) and on days 7 and 14. Animals dying intercurrently were weighed upon discovery of death. Gross necropsies were performed on all animals which died during the study. On day 14, all surviving animals were sacrificed and gross necropsy examinations were performed.

Species/strain:	Sprague-Dawley rats
No. Animals:	5 male and 5 females (for exposure and control)
Dose:	0.353 mg/L or 38.7 ppm (nominal)
Vehicle:	undiluted
Exposure Period:	6 hours
Post-exposure observations:	14 days
GLP:	Yes
Year:	1987
Results:	Chamber air mean temperature was 75°F and the mean relative humidity was 40% for the exposure group. The mean temperature was 76°F and the mean relative humidity was 44% for the control group. A total of 2.54 g of cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester was delivered in a total volume of 7200 L of air, yielding a nominal concentration exposure of 0.353 mg/L, approximately 38.7 ppm. The mean measured airborne test material concentration was 108 ppm “methane equivalents”. The recorder trace of the analyzer output indicated that there was a constant, relatively stable output of vapor from the evaporation system throughout the exposure. Since the correlation of responses between “methane equivalents” and actual concentration of the test material is unknown, this measurement serves only to show stability of the airborne concentration of test material and the nominal concentration is used as the best estimate of exposure concentration.

There were no deaths during the study. Clinical signs noted among test rats during and shortly after exposure included squinting eyes, excessive lacrimation, red perinasal fur and irregular breathing patterns. All rats had

recovered by study day 1 and remained healthy until termination. All rats gained weight during the study except for one rat. There were no gross treatment-related lesions observed in any animal at necropsy. One rat in the exposure group had a herniated liver.

This finding was judged to be a developmental anomaly commonly found in this strain of rat and is not considered to be related to treatment. The test material produced only transient signs of irritation at an essentially saturated vapor concentration. Therefore, an acute inhalation toxicity hazard is extremely unlikely.

Data Quality: 2e

References: FMC 39338 Technical, Acute Inhalation Toxicity Screen in Rats, FMC Toxicology Laboratory, FMC Study Number A85-1657

## 5.2 REPEATED DOSE TOXICITY

Remarks: Requirement waived for closed system intermediates.

## 5.3 GENETIC TOXICITY IN VITRO

### 5.3.1 SOURCE #1

Test Substance: Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester

Method: EPA Guideline, 1983

Type: *Salmonella*/Mammalian-Microsome Plate Incorporation Mutagenicity Assay (Ames Test). Each treatment was run in triplicate with and without metabolic activation by rat liver microsomes. Induced with Aroclor 1254. Solubility and toxicity to bacterial were determined prior to the assay. Positive controls included sodium azide, 9-aminoacridine, and 2-nitrofluorene without S9 and 2-anthramine with S9. The negative control was the vehicle, DMSO.

System of Testing: *S. typhimurium* strains TA98, TA100, TA1535, TA1537 and TA1538

Concentration: 50, 100, 250, 500 and 1000 ug/plate with and without S9

Metabolic Activation: With and without S9

GLP: Yes

Year: 1986

Results: The test article did not cause a positive response in any of the tester strains with or without metabolic activation. The positive controls gave the expected increase in mutant frequency. The positive and negative controls met the criteria for a valid test. The test article is considered not mutagenic in this assay.

Data Quality: 1a

References: "Salmonella/Mammalian-Microsome Plate Incorporation Mutagenicity Assay (Ames test)," FMC Corporation Genetic Toxicology Laboratory, FMC Study Number A84-1451. April 6, 1986; Mutation Research 48, 121-130, 1977

### 5.3.2 SOURCE #2

Test Substance: Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester (98.7% pure)

Method: OECD 473

Type: Chromosomal aberration

System of Testing: Cultured Chinese Hamster Lung (CHL) cells in the presence (+S) and absence (-S) of metabolic activation system (S-9 mix).

Concentration: 6-hr treatment - 0, 100, 300, 500, 700, 900 µM with S9 activation  
6-hr and 24-hr treatment - 0, 37.5, 75, 150, and 300 µM without S9 activation

Metabolic Activation: With and without S9 activation.

GLP: Yes

Year: 2004

Results: Methyl D. V. Ester was evaluated for mutagenicity with the chromosome aberration method using Chinese Hamster Lung cells in the presence and absence of a metabolic activation system. Three day old cell cultures were exposed to MDVE or control solution under the following treatment conditions:

1. 6 hour treatment in the presence of S-9 mix followed by an 18-hour recovery,
2. 6 hour treatment in the absence of S-9 mix followed by an 18 hour recovery, and
3. 24 hour continuous treatment in the absence of S-9 mix.

Dimethylsulfoxide (DMSO) was used as the negative control and cyclophosphamide (CPA) and ethylmethanesulfonate (EMS) was used for positive controls. The highest concentration used in the study was determined in a preliminary range-finding study. Vehicle and positive control groups were included in each of the treatment conditions. There were no statistically significant increases in the number of aberrant metaphases with or without activation in cultures exposed to MDVE at any concentration. MDVE did not induce structural chromosomal aberrations at the concentration range tested in cultured CHL cells.

Data Quality: 1a

References: Methyl D. V. Ester (FMC 39338): Test for chemical induction of chromosome aberrations in cultured Chinese Hamster Lung (CHL) cells [FMC study number A2004-5821].

#### 5.4 REPRODUCTION/DEVELOPMENTAL TOXICITY SCREENING

Test Substance:	Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, methyl ester (98.7% pure)
Method:	OECD 421
GLP:	Yes
Year:	2004
Species:	Rat
Strain:	SPF Sprague-Dawley (Crj:CD®(SD)IGS.BR) rats
Route of Administration:	Oral gavage in corn oil
Doses:	0, 50, 450 and 900 mg/kg/day
Sex:	Male and Female
Exposure Period:	Males – from 2 weeks before mating to end of mating period Females – from 2 weeks before mating through gestation and to day 3 post partum.
Frequency of Treatment:	Once per day
Control and Treatment Groups:	Yes
Duration of Test:	Males – 28 days Females – 54 days
Statistical Methods:	Statistical analysis was performed by comparing the treatment groups with the vehicle control group using Path/Tox system (Xybio Medical System Co., NJ, USA). The pregnant dams or the litters were used as the unit of comparison. Parametric data such as body weight, food consumption, organ weight, and fetal body weight were subjected to one-way analysis of variance (ANOVA), and Scheffe's multiple comparison test was conducted when analytical results were significant. Non-parametric data such as the number of corpora lutea, total implantations, and live/dead fetuses were statistically evaluated using the Kruskal-Wallis ANOVA, followed by Scheffe's multiple comparison test. A difference was considered statistically significant at $p < 0.05$ or $p < 0.01$ .
Results:	There was a high incidence of salivation in both sexes at the 450 and 900 mg/kg dose levels. Two moribund females were sacrificed at 900 mg/kg. There were no treatment-related changes in body weight, food consumption, necropsy findings, and male reproductive organ weights or histopathological findings. An increase in perinatal deaths, decreased number and body weights of live young at birth, and litter size were observed at the high dose (900 mg/kg). No treatment-related effect was seen in gestation length, viability index, sex ratio, number of pups with gross lesions, or pups with abnormally low body weights. No adjustment was made to dose levels based on purity. Based on these results, the NOAEL was 450 mg/kg .
Data Quality:	1a
References:	A Reproductive/Developmental Toxicity Screening Test of Oral Administration of Methyl D.V. Ester (FMC39338) in Rats. [FMC Study number A2004-5820]

## CRITERIA FOR RELIABILITY CODES

(Adapted from Klimisch et al 1997)

### Code of Reliability

### Category or reliability

#### **1**

#### **Reliable without restriction**

1a

GLP guideline study (OECD, EC, EPA, FDA, etc.)

1b

Comparable to guideline study

1c

Test procedure in accordance with generally accepted scientific standards and described in sufficient detail

#### **2**

#### **Reliable with restrictions**

2a

Guideline study without detailed documentation

2b

Guideline study with acceptable restrictions

2c

Comparable to guideline study with acceptable restrictions

2d

Test procedure in accordance with national standard methods with acceptable restrictions

2e

Study well documented, meets generally accepted scientific principles, acceptable for assessment

2f

Accepted calculation method

2g

Data from handbook or collection of data

#### **3**

#### **Not reliable**

3a

Documentation insufficient for assessment

3b

Significant methodological deficiencies

3c

Unsuitable test system

#### **4**

#### **Not assignable**

4a

Abstract

4b

Secondary literature

4c

Original reference not yet available

4d

Original reference not yet translated

4e

Documentation insufficient for assessment