



201-13406

The Dow Chemical Company
Midland, Michigan 48674

2020 DOW CENTER
December 18, 2001

Ms. Christine Todd Whitman
Administrator
U.S. Environmental Protection Agency
P.O. Box 1473
Merrifield, VA 22116

Dear Ms. Whitman:

CHEMICAL RIGHT TO KNOW – HPV CHALLENGE PROGRAM

On behalf of The Dow Chemical Company, I am pleased to submit the robust summaries in IUCLID format for Ethyl Monochloroacetate (Cas No.: 105-39-5). As requested, the test plan has been posted onto the U.S. HPV Chemical Tracking System. All documents are Adobe Acrobat (pdf) files.

We understand this information will be posted on the internet for comments for a period of 120 days. Please forward comments to me at the following address:

Ms. Connie L. Deford
The Dow Chemical Company
2020 Dow Center
Midland, MI 48674

Sincerely,

Connie L. Deford
Global Environment, Health & Safety Manager
(989) 636-6978

AR201-13406A

**HIGH PRODUCTION VOLUME (HPV)
CHEMICAL CHALLENGE PROGRAM**

TEST PLAN

For

ETHYL MONOCHLOROACETATE

Prepared by:

The Dow Chemical Company

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December, 2001

EXECUTIVE SUMMARY

The Dow Chemical Company hereby submits for review and public comment the test plan for ethyl monochloroacetate (EMCA) (CAS No. 105-39-5), which we have classified as a closed-system intermediate, under the Environmental Protection Agency's (EPA) High Production Volume (HPV) Chemical Challenge Program. It is the intent of The Dow Chemical Company to primarily use existing data and scientific judgment and analyses to adequately characterize the SIDS (Screening Information Data Set) human health, environmental fate and effects, and physicochemical endpoints for this chemical. Additional data will be collected under the HPV Challenge Program as defined in this test plan.

Please note that we are aware that there is another importer of EMCA into the United States. We have tried to reach this company to determine if they were interested in joining with Dow in our commitment to the HPV Chemical Challenge Program. Further, we asked them to assess whether or not their import, handling, and use of EMCA would fulfill the criteria outlined by EPA for a closed-system intermediate. Unfortunately, the company declined to respond to our invitation and did not provide any information on their handling or use of EMCA.

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TEST PLAN FOR ETHYL MONOCHLOROACETATE

I. INTRODUCTION

The Dow Chemical Company has voluntarily committed to develop and/or summarize screening level human health effects, environmental effects and fate, and physicochemical test data for ethyl monochloroacetate under the Environmental Protection Agency's (EPA's) High Production Volume (HPV) Challenge Program.

This plan identifies the chemical and its CAS number, identifies existing data of adequate quality for the chemical, provides justification for why additional toxicity data is not needed to characterize human health effects, and describes additional testing to be conducted for the chemical under the Program

II. DESCRIPTION OF ETHYL MONOCHLOROACETATE

A. The Chemical

Ethyl monochloroacetate (CAS No. 105-39-5) is a member of a group of chemicals referred to as esters of monocarboxylic halogenated acids. The halogenated acetates are used primarily as intermediates in organic synthesis processes. As is typical in this group, ethyl monochloroacetate is a colorless liquid with a relatively high density, good solubility in water, and good stability to hydrolytic processes. Halogenated acetates tend to have similar toxicity profiles, with a primary effect being pulmonary edema, as well as lacrimatory and irritant properties.

Table 1. Chemical/physical properties Ethyl *Monochloroacetate*

<i>Chemical Abstract Number</i>	<i>105-39-5</i>
<i>Molecular formula</i>	<i>C₄H₇ClO₂</i>
<i>Molecular weight</i>	<i>122.56</i>
<i>Physical State</i>	<i>Clear, Colorless liquid</i>
<i>Melting Point</i>	<i>-26°C</i>
<i>Boiling point</i>	<i>144 °F @ 760 mmHg</i>
<i>Vapor pressure</i>	<i>4.5 hPa @20°C</i>
<i>Water Solubility</i>	<i>20 g/l @ 19.8°C</i>
<i>Specific Gravity</i>	<i>1.1585g/cm³ @ 20°C</i>
<i>Flash Point</i>	<i>53° C</i>

The health hazards to humans can be summarized as follows:

Eyes: Liquid EMCA and its vapors can cause severe irritation and corneal injury sufficient to result in permanent impairment.

Skin: Prolonged or repeated exposure may produce severe irritation with burns, if confined, and may be absorbed through the skin in acutely toxic amounts to the extent that systemic injury may be sufficient to cause death.

Ingestion: There is little likelihood that ingestion will occur in routine industrial applications. Nevertheless, small amounts ingested incidentally to industrial handling are not likely to cause injury. Ingestion of large amounts would likely be injurious to the mouth, throat, and gastrointestinal tract.

Inhalation: Exposure to vapors may result in severe consequences and intolerable irritation to the respiratory passage.

III. TEST PLAN RATIONALE

A. Classification of the Chemical as a Closed-System Intermediate

1. Requirements

Classification of ethyl monochloroacetate as a closed-system intermediate under the EPA HPV program is dependent upon a number of criteria outlined by EPA. The Dow Chemical Company asserts that ethyl monochloroacetate should be regarded as a closed-system intermediate, based on satisfaction of these criteria. In the following paragraphs, we have provided information on the extremely limited potential for exposure during manufacturing, transport and processing.

2. Satisfaction of Requirements

a. Review of Manufacture / Transport / Consumption:

Ethyl Monochloroacetate (EMCA) is produced in a single facility within The Dow Chemical Company's Michigan Operations Site located in Midland, Michigan. EMCA is manufactured from chloroacetyl chloride in a completely closed system. The sole use of EMCA is as an on-site intermediate in the production of another chlorinated derivative, manufactured within the same manufacturing site where EMCA is produced. After the EMCA is manufactured, it is placed in a storage tank, which is vented to a caustic scrubber, located in a diked area. EMCA is transferred to the downstream facility via pipeline. There is no offsite transfer of this material.

b. Environmental Fate

The potential for environmental exposure to EMCA is negligible. There are minimal releases to the air, which occur through both point source and fugitive releases, but these represent a fraction of the EMCA produced. There are no releases to water or land unless a major plant upset occurred. In case of a plant upset or storage tank leak, EMCA would be contained in the dike that surrounds the manufacturing and storage area

Since the EMCA is consumed entirely as an intermediate, the downstream processing will result in yet a smaller fraction of air emissions than during manufacturing. As the residual

level of EMCA in its downstream product is non-detectable (L.O.D. - 1 ppm level), there is essentially no potential for environmental exposure through its use.

c. Human Exposure

The potential for human exposure is also extremely low. The total number of workers within our production and processing facility is less than 20. Due to the inherent irritant nature of EMCA, personal protective equipment is worn during production, maintenance, distribution and processing to ensure no personal contact. During normal operation, this would include goggles and hard hats. During an operation, such as a line opening, where there is a potential for EMCA to be present, the protective equipment would include goggles, face shield, hard hat, protective full rubber suit, boots and a full-face respirator. Suitable positive-pressure self-contained breathing apparatus would be used for longer-term exposure in emergency situations such as a spill clean up.

Available monitoring data from the production of EMCA, which is conducted periodically, indicates that the exposures are well below the industrial hygiene guideline established for EMCA. The 8-hour Time-Weighted Average exposure limit for EMCA is 0.1ppm, Skin.

A summary of the actual monitoring data, from the activities, which are expected to have the greatest potential for worker exposures, is included in the following table. During these activities, personal protective equipment is worn.

WORKER EXPOSURE DATA FOR EMCA

ACTIVITY	MONITORING DATA	SAMPLE DURATION	COMMENT
Collected Process Sample	ND (0.02 ppm)	6 min.	Personal Sample
Collected Process Sample	0.08 ppm	6 min.	Personal Sample
Outdoors near Sample Collection Box	0.07 ppm	5 min.	Area Sample

As the residual level of EMCA in the downstream product is non-detectable (L.O.D. – 1ppm), there is essentially no potential for worker or public exposure during processing. There is no potential for public exposure unless there would be a significant manufacturing plant upset or catastrophic event. We have a program in place to conduct extensive root cause investigations if any such incidents were to occur and to develop a corrective action plan to prevent reoccurrence.

3. Conclusion

The Dow Chemical Company believes that the information above fully satisfies the EPA's criteria for closed-system intermediates. Further, the above information suggests that there appears to be little additional action that could be taken to prevent any further exposure, as the potential exposure opportunity is extremely limited.

B. Human Health Effects

There are six mammalian toxicity endpoints in the HPV Program (Results summarized in the table on Page 7):

- Acute Toxicity
- Repeated Dose Toxicity
- Genetic Toxicity *In Vitro*
- Genetic Toxicity *In Vivo*
- Reproductive Toxicity
- Developmental Toxicity

Published and unpublished data, as detailed in the attached Robust Summaries, satisfy the requirements of Acute, Repeated Dose, and *In Vitro* Genetic Toxicity endpoints. Since *in vitro* genetic toxicity endpoints are negative, *in vivo* testing has not been addressed.

As EMCA satisfies the EPA's criteria as a closed-system intermediate, the only data gap that exists is for a Developmental Toxicity study. Based on our demonstration above that the potential for any human and environmental exposure is highly unlikely and that repeated human and environmental exposure are even less likely, we do not believe that a development toxicity test is justified. Further, the corrosive nature of the compound will limit the dose that can be tolerated by the animals, which limits the potential to show any adverse effect if such a study were conducted.

The attached Robust Summaries provide adequate data to characterize the human health effects endpoints under the Program.

C. Ecotoxicity

There are three aquatic toxicity endpoints in the HPV Program:
(Results summarized in the table on Page 7)

- Acute Toxicity to Fish
- Acute Toxicity to Aquatic Invertebrates
- Toxicity to Algae (Growth Inhibition)

Published and unpublished data, as detailed in the attached Robust Summaries, satisfies requirements for Acute Toxicity to Fish and Aquatic Invertebrates. To satisfy the remaining requirement, a test for acute toxicity to algae is planned, in compliance with OECD Guideline

201. The recommended testing, in conjunction with existing data, will provide adequate data to characterize ecotoxicity endpoints under the Program.

D. Environmental Fate

(Results summarized in the table on Page 7)

Predictive models were used to develop meaningful data for chemicals that are gaseous at relevant environmental temperatures and pressures. The environmental fate data include:

- Photodegradation
- Stability in Water (Hydrolysis)
- Transport and Distribution (Fugacity)
- Biodegradation

1. Photodegradation

Photodegradation was estimated using models accepted by the EPA. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows)¹ is used by The Dow Chemical Company. This program calculates a chemical half-life based on an overall OH reaction rate constant, a 12-hr day, and a given OH concentration. This calculation was performed for ethyl monochloroacetate, as detailed in the attached Robust Summaries.

2. Stability in Water (Hydrolysis Testing and Modeling)

Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters⁴. Stability in water can be measured³ (EPA identifies OECD test guideline 111 as a test method). Experimentally determined data for ethyl monochloroacetate, as referenced in Howard² and as detailed in the attached Robust Summaries is available.

3. Chemical Transport and Distribution In The Environment (Fugacity Modeling)

The US EPA has acknowledged that computer modeling techniques are an appropriate approach to estimating chemical partitioning (fugacity is a calculated endpoint and is not measured). A widely used fugacity model is the EQC (Equilibrium Criterion) model⁵. EPA cites the use of this model in its document titled *Determining the Adequacy of Existing Data*³, which was prepared as guidance for the HPV Program.

The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. This model has been used to calculate distribution values for ethyl monochloroacetate. A computer model, EPIWIN - version 3.02¹, has been used to calculate the properties needed to run the Level I EQC

model. The distribution values for ethyl monochloroacetate are detailed in the attached Robust Summaries.

4. Biodegradation Testing

Biodegradation values for ethyl monochloroacetate, as detailed in the attached Robust Summaries, were experimentally determined using OECD Guideline 302B.

E. Physicochemical Properties

(Results are summarized in the “Description of the Chemical” on page 1.)

The physicochemical properties include:

- Melting Point
- Boiling Point
- Vapor Pressure
- Octanol/Water Partition Coefficient

Data for physicochemical properties will be summarized from various resources and detailed in the attached Robust Summaries.

IV. TEST PLAN SUMMARY

The following testing will be conducted for ethyl monochloroacetate:

- Conduct an algal toxicity study.

For reasons indicated in the above paragraphs, we do not believe additional data needs to be generated beyond this algal toxicity study. Due to the manner in which the chemical is manufactured, distributed, and processed; the product stewardship measures taken to prevent exposure; and existing human/environmental data, we believe that our workers, the public and the environment are well protected from exposure to EMCA. Most importantly, we do not believe that generation of any additional data, especially developmental toxicity testing, will impact our handling or product stewardship practices. Due to the acute hazards of this compound, our process and procedures are designed to prevent any exposure to our workers and the public.

Test Plan for Ethyl monchloroacetate

Endpoint	Data Availability	Acceptable (Reliability)	Planned Testing
Acute Toxicity	Oral LD50: 50 – 200 mg/kg (rat) Oral LD50: 350 mg/kg (mouse) Dermal LD50: 161 mg/kg (rat) Dermal LD50: 230 - 335 mg/kg (rabbit) Dermal Irritation: Moderately Irritating (rabbit) Eye Irritation: Highly Irritating (rabbit)	Acceptable (1)	None
Repeated Dose Toxicity (Carcinogenicity: 580 days)	Negative (See Robust Summary for details)	Acceptable (2)	None
Genetic Toxicity <i>In Vitro</i>	Ames – negative Genetic mutation - negative	Acceptable (1)	None
Genetic Toxicity <i>In Vivo</i>	Not available	Not necessary	None
Reproductive Toxicity	Not available	Not required	None
Developmental Toxicity	Not available	Not necessary	None
Acute Toxicity to Fish	LC50 1.48 mg/L (OECD 203)	Acceptable (2)	None
Acute Toxicity to Aquatic Invertebrates	EC50 3.3 mg/L (DIN 38412)	Acceptable (2)	None
Toxicity to Algae (Growth Inhibition)	Not available	To Be Conducted	Algal growth inhibition study
Photodegradation	50% after 15.7 days (calculated)	Acceptable (1)	None
Stability in Water (Hydrolysis)	Half life: pH 7 – 9.1 day @25°C pH 8 – 21.8 hrs @25° C (calculated)	Acceptable (2)	None
Transport and Distribution (Fugacity)	Level I: Air – 45.1 Water – 54.5 Soil – 0.42 (calculated)	Acceptable (1)	None
Biodegradation	75% after 28 days (OECD 301 F) 93% after 13 days (OECD 302 B)	Acceptable (1)	None

REFERENCES

1. EPIWIN. 1999. Estimation Program Interface for Windows, version 3.02. Syracuse Research Corporation, Syracuse, NY, USA.
2. Howard, P. H. 1997. Handbook of Environmental Fate and Exposure Data. Vol. 5, pp. 196-200.
3. US EPA. 1999. Determining the Adequacy of Existing Data. OPPT, EPA.
4. Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.
5. Mackay, D., A. Di Guardo, S. Paterson, and C. E. Cowan. 1996. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environ. Toxicol. Chem. 15:1627-1637.

I U C L I D

Data Set

RECEIVED
OPPT NCIC
2001 DEC 21 PM 2:21

Existing Chemical : ID: 105-39-5
CAS No. : 105-39-5
EINECS Name : ethyl chloroacetate
EINECS No. : 203-294-0
TSCA Name : Acetic acid, chloro-, ethyl ester
Molecular Formula : C4H7ClO2

Producer Related Part
Company : The Dow Chemical Company
Creation date : 03.11.2000

Substance Related Part
Company : The Dow Chemical Company
Creation date : 03.11.2000

Memo :

Printing date : 17.12.2001
Revision date :
Date of last Update : 17.12.2001

1. General Information

Id 105-39-5
Date 17.12.2001

1.0.1 OECD AND COMPANY INFORMATION

Type :
Name : The Dow Chemical Company
Partner :
Date :
Street : 2020 Building
Town : 48674 Midland, MI
Country : United States
Phone : 989-636-1000
Telefax :
Telex :
Cedex :
17.12.2001

1.0.2 LOCATION OF PRODUCTION SITE

Name of Plant : Michigan Operations Site, The Dow Chemical Company
Street :
Town : 48674 Midland, MI
Country : United States
Phone : 989-636-1000
Telefax :
Telex :
Cedex :
Remark : Ethyl Monochloroacetate (EMCA) is produced in a single facility within The Dow Chemical Company's Michigan Operations Site located in Midland, Michigan. EMCA is manufactured from chloroacetyl chloride in a completed closed system. The sole use of EMCA is as an on-site intermediate in the production of another chlorinated derivative, manufactured within several blocks of the production of EMCA. Upon completion of production, the EMCA is placed in a storage tank, which is vented to a caustic scrubber. EMCA is transferred to the downstream plant via pipeline. There is no offsite transfer of this material.
17.12.2001

1.0.3 IDENTITY OF RECIPIENTS

1.1 GENERAL SUBSTANCE INFORMATION

Substance type : organic
Physical status : liquid
Purity : % w/w
Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
10.02.2000

1.1.0 DETAILS ON TEMPLATE

1.1.1 SPECTRA

1.2 SYNONYMS

Acetic acid, chloro-, ethyl ester
Acetic acid, chloro-, ethyl ester (6Cl, 8Cl, 9Cl)
Chloroacetic acid ethyl ester
Ethyl 2-chloroacetate
Ethyl chloroacetate
Ethyl chloroethanoate
Ethyl monochloracetate
Ethyl monochloroacetate

1.3 IMPURITIES

1.4 ADDITIVES

1.5 QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.7 USE PATTERN

1.7.1 TECHNOLOGY PRODUCTION/USE

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUES

Type of limit	: MAK (DE)
Limit value	: 1 ml/m ³
Remark	: Spitzenbegrenzung: Kategorie 1; Gefahr der Hautresorption
Source	: Hoechst AG Frankfurt/Main Clariant GmbH Frankfurt am Main EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

21.01.1997 (1)

1.9 SOURCE OF EXPOSURE

1.10.1 RECOMMENDATIONS/PRECAUTIONARY MEASURES

1.10.2 EMERGENCY MEASURES

1. General Information

Id 105-39-5
Date 17.12.2001

1.11 PACKAGING

1.12 POSSIB. OF RENDERING SUBST. HARMLESS

1.13 STATEMENTS CONCERNING WASTE

1.14.1 WATER POLLUTION

1.14.2 MAJOR ACCIDENT HAZARDS

1.14.3 AIR POLLUTION

1.15 ADDITIONAL REMARKS

1.16 LAST LITERATURE SEARCH

1.17 REVIEWS

1.18 LISTINGS E.G. CHEMICAL INVENTORIES

2.1 MELTING POINT

Value : = -26.6 °C
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
10.12.1993 (10)

Value : ca. -26 °C
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
10.12.1993 (3) (4)

Value : ca. -26 °C
Remark : Erstarrungspunkt
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
21.01.1997 (8) (1)

2.2 BOILING POINT

Value : = 144.2 °C at
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
10.12.1993 (11)

Value : = 144.2 °C at
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
10.12.1993 (11)

Value : = 144.2 °C at
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
10.12.1993 (11)

2.3 DENSITY

Type : density
Value : 1.15 - 1.155 g/cm³ at 20° C
Method : other: DIN 51751, ASTM D 1298-90
Year :
GLP :
Test substance :
Source : Hoechst AG Frankfurt 80
 Rhone-Poulenc Chimie Courbevoie Cedex
 Hoechst AG Frankfurt 80
 Hoechst AG Frankfurt/Main
 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
 10.12.1993 (3) (4)

Type : density
Value : 1.15 - 1.155 g/cm³ at 20° C
Method : other: DIN 51751, ASTM D 1298-90
Year :
GLP :
Test substance :
Source : Hoechst AG Frankfurt/Main
 Clariant GmbH Frankfurt am Main
 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
 21.01.1997 (8) (1)

Type : density
Value : = 1.1585 g/cm³ at 20° C
Source : Hoechst AG Frankfurt 80
 Rhone-Poulenc Chimie Courbevoie Cedex
 Hoechst AG Frankfurt 80
 Hoechst AG Frankfurt/Main
 Hoechst AG Frankfurt/Main
 Clariant GmbH Frankfurt am Main
 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
 10.12.1993 (11)

Type : density
Value : = 1.159 g/cm³ at 20° C
Source : Hoechst AG Frankfurt 80
 Rhone-Poulenc Chimie Courbevoie Cedex
 Hoechst AG Frankfurt 80
 Hoechst AG Frankfurt/Main
 Hoechst AG Frankfurt/Main
 Clariant GmbH Frankfurt am Main
 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
 10.12.1993 (10)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : = 4.5 hPa at 20° C
Source : Hoechst AG Frankfurt 80
 Rhone-Poulenc Chimie Courbevoie Cedex
 Hoechst AG Frankfurt 80

2. Physico-Chemical Data

Id 105-39-5
Date 17.12.2001

10.12.1993
Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
(3) (4)

Value : = 4.5 hPa at 20° C
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
21.01.1997 (8) (1)

Value : = 4.8 hPa at 20° C
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
10.12.1993 (11)

Value : = 8.8 hPa at 30° C
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
10.12.1993 (11)

Value : = 13.3 hPa at 37.5° C
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
10.12.1993 (10)

2.5 PARTITION COEFFICIENT

Log pow : = 1.12 at ° C
Method other (calculated): EPIWIN V1.0, Syracuse Research Corporation, N.Y.
1994

Year :
GLP :
Test substance :
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
14.12.1995 (12)

Log pow : = 1.13 at ° C
Method other (calculated): Leo, Hansch: CLOGP3, Release 3.42, Pomona College,
Clermont CA
Year : 1986
GLP :
Test substance :
Source : Hoechst AG Frankfurt 80

2. Physico-Chemical Data

Id 105-39-5
Date 17.12.2001

10.12.1993
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA) (13)

Log pow : = 1.13 at ° C
Method : other (calculated): Leo, Hansch: CLOGP3, Release 3.42, Pomona College, Clermont CA

Year : 1986

GLP :

Test substance :

Source :

Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA) (14)

26.09.1994

2.6.1 WATER SOLUBILITY

Value : = 20 g/l at 19.8 ° C
Qualitative :
Pka : at 25 ° C
PH : at and ° C
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA) (3) (15)

10.12.1993

Value : = 20 g/l at 19.8 ° C
Qualitative :
Pka : at 25 ° C
PH : at and ° C
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA) (8) (1) (15)

21.01.1997

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value : = 53 ° C
Type : closed cup
Method : other: DIN 51758
Year :
GLP :
Test substance :
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA) (3) (4)

10.12.1993

Value : = 53 ° C

2. Physico-Chemical Data

Id 105-39-5
Date 17.12.2001

Type : closed cup
Method : other: DIN 51758
Year :
GLP :
Test substance :
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
21.01.1997 (8) (1)

2.8 AUTO FLAMMABILITY

Value : = 452 °C at
Method : other: DIN 51794, ASTM E 659-89
Year :
GLP :
Test substance :
Remark : Zundtemperatur
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
21.01.1997 (8) (1)

2.9 FLAMMABILITY

Result : flammable
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
21.01.1997 (1)

2.10 EXPLOSIVE PROPERTIES

Result : other
Remark : Untere Explosionsgrenze (in Luft bei 1013mbar): 2,6 Vol.-%
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
21.01.1997 (8) (1)

2.11 OXIDIZING PROPERTIES

2.12 ADDITIONAL REMARKS

Remark : Dynamische Viskositaet bei 20 Grad C: 1.27 mPas (Methode:
DIN 51562, ASTM D 445-88)
Zuendtemperatur: 452 Grad C (Methode: DIN 51794,
ASTM E 659-89)
Untere Explosionsgrenze (in Luft bei 1013 mbar): 2.6 Vol.-%
Gefaehrliche Zersetzungsprodukte: Chlorwasserstoff,
Monochloressigsaeure
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80

3. Environmental Fate and Pathways

Id 105-39-5
Date 17.12.2001

3.1.1 PHOTODEGRADATION

Type : air
Light source :
Light spect. : nm
Rel. intensity : based on Intensity of Sunlight
Indirect photolysis
Sensitizer : OH
Conc. of sens. : 500000 molecule/cm3
Rate constant : = .0000000000010238 cm3/(molecule*sec)
Degradation : = 50 % after 15.7 day
Deg. Product :
Method : other (calculated): EPIWIN V1.0, Syracuse Research Corporation, N.Y. 1994
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Remark : No further information available.
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions
30.08.2001 (12)

Type : air
Light source :
Light spect. : nm
Rel. intensity : based on Intensity of Sunlight
Indirect photolysis
Sensitizer : OH
Conc. of sens. : 500000 molecule/cm3
Rate constant : = .00000000000144 cm3/(molecule*sec)
Degradation : = 50 % after 11.1 day
Deg. Product :
Method : other (calculated): Atkinson
Year : 1988
GLP :
Test substance : as prescribed by 1.1 - 1.4
Remark : No further information available.
Source : Hoechst AG Frankfurt 80
Rhône-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions
30.08.2001 (17)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at degree C
t1/2 pH7 : = 9.1 day at 25 degree C
t1/2 pH9 : at degree C
t1/2 pH 8 : = 21.8 hour(s) at 25 degree C
Deg. Product :
Method : other: EPIWIN V1.0, Syracuse Research Corporation, N.Y. 1994
Year :

3. Environmental Fate and Pathways

Id 105-39-5
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GLP :
Test substance :
Remark : No further information available.
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (1) valid without restriction
30.08.2001 (12)

3.1.3 STABILITY IN SOIL

3.2 MONITORING DATA

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media : other: mathematical modeling
Air (level I) : 45.1
Water (level I) : 54.5
Soil (level I) : .42
Biota (level II / III) : 0
Soil (level II / III) : 2.2
Method : other: Mackay Level I/III fugacity modeling
Year : 2001
Source : The Dow Chemical Company
Test condition : Required Input Values for Level I/III Modeling of Ethyl Chloroacetate

Property	Value
Chemical Type	1
Molecular Mass (g/mol)	122.55
Water Solubility (g/m3)	19400
Vapor Pressure (Pa)	649
Melting Point (0C)	-23
Estimated Henry's Law Constant (H) (Pa m3/mol) = (J/mol)	4.1
Kaw	
Air-Water Partition Coefficient	1.66E-3
Log Kow	
Octanol-Water Partition Coefficient	0.94
Temperature (0C)	25
Amount of Chemical input to the System (kg)	100,000

Reliability : (1) valid without restriction
17.12.2001 (18)

Type : adsorption
Media : water - soil
Air (level I) :
Water (level I) :
Soil (level I) :
Biota (level II / III) :
Soil (level II / III) :
Method : other: EPIWIN V1.0, Syracuse Research Corporation, N.Y. 1994
Year :
Result : Koc (berechnet): 11.8
Source : Hoechst AG Frankfurt/Main

3. Environmental Fate and Pathways

Id 105-39-5
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Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (1) valid without restriction
17.12.2001 (12)

Type : volatility
Media : water - air
Air (level I) :
Water (level I) :
Soil (level I) :
Biota (level II / III) :
Soil (level II / III) :
Method : other: EPIWIN V1.0, Syracuse Research Corporation, N.Y. 1994
Year :
Result : Henry Programm Results:

Bond Estimation Method: 8.20E-005 atm-m3/mole
Group Estimation Method: 4.77E-005 atm-m3/mole

Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (1) valid without restriction
30.08.2001 (12)
17.12.2001

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, domestic, non-adapted
Concentration : 83.3mg/l related to Test substance
related to

Contact time :
Degradation : = 75 % after 28 day
Result : readily biodegradable
Kinetic of test substance : 3 day = 22 %
8 day = 60 %
14 day = 70 %
21 day = 73 %
%

Deg. Product Method : OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year : 1996
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (1) valid without restriction
17.11.2000 Guideline-Studie (19)

3. Environmental Fate and Pathways

Id 105-39-5
Date 17.12.2001

Type : aerobic
Inoculum : activated sludge, industrial, non-adapted
Concentration : 1040mg/l related to Test substance related to
Contact time :
Degradation : = 93 % after 13 day
Result :
Kinetic of test substance : 3 hour(s) < 10 %
%
3 day < 10 %
6 day = 40 %
8 day = 61 %
Deg. Product Method : OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year : 1986
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : Abbau durch nichtbiologische Vorgaenge: ca. 30 %
Source : Hoechst AG Frankfurt 80
Rhône-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (1) valid without restriction
30.08.2001 (20)

Type : aerobic
Inoculum : activated sludge, industrial, non-adapted
Concentration : 520mg/l related to Test substance related to
Contact time :
Degradation : = 93 % after 8 day
Result :
Kinetic of test substance : 3 hour(s) < 10 %
%
3 day = 11 %
6 day = 83 %
%
Deg. Product Method : OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year : 1986
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : Abbau durch nichtbiologische Vorgaenge: ca. 30 %
Source : Hoechst AG Frankfurt 80
Rhône-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (1) valid without restriction
30.08.2001 (20)

Type : aerobic
Inoculum : activated sludge, industrial, non-adapted
Concentration : 1040mg/l related to Test substance related to
Contact time :

3. Environmental Fate and Pathways

Id 105-39-5
Date 17.12.2001

Degradation Result : = 93 % after 13 day
:
Kinetic of test substance : 3 hour(s) < 10 %
:
%
3 day < 10 %
6 day = 40 %
8 day = 61 %

Deg. Product Method :
: OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year : 1986
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : Abbau durch nichtbiologische Vorgange: ca. 30 %
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (1) valid without restriction
30.08.2001 (21)

Type : aerobic
Inoculum : activated sludge, industrial, non-adapted
Concentration : 520mg/l related to Test substance related to

Contact time :
Degradation Result : = 93 % after 8 day
:
Kinetic of test substance : 3 hour(s) < 10 %
:
%
3 day = 11 %
6 day = 83 %
%

Deg. Product Method :
: OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year : 1986
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : Abbau durch nichtbiologische Vorgange: ca. 30 %
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (1) valid without restriction
30.08.2001 (21)

Type : aerobic
Inoculum : activated sludge, industrial, non-adapted
Contact time :
Degradation Result : > 95 % after 15 day
:
Kinetic of test substance : 5 day = 15 %
:
10 day = 82 %
%
%
%

Deg. Product Method :
: OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year : 1979

3. Environmental Fate and Pathways

Id 105-39-5
Date 17.12.2001

GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : Abbau durch nichtbiologische Vorgaenge: <10 %
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (1) valid without restriction
30.08.2001 (22)

Type : aerobic
Inoculum : activated sludge, industrial, non-adapted
Contact time :
Degradation : > 95 % after 15 day
Result :
Kinetic of test substance : 5 day = 15 %
10 day = 82 %
%
%
%

Deg. Product Method :
: OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year : 1979
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : Abbau durch nichtbiologische Vorgange: <10 %
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (1) valid without restriction
30.08.2001 (23)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : static
Species : Brachydanio rerio (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring : no
LC0 : = 1
LC50 : = 1.48
LC100 : = 2.2
Method : OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year : 1989
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : No further information available.
Source : Hoechst AG Frankfurt 80
 Rhone-Poulenc Chimie Courbevoie Cedex
 Hoechst AG Frankfurt 80
 Hoechst AG Frankfurt/Main
 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions
 30.08.2001 (24)

Type : static
Species : Brachydanio rerio (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring : no
LC0 : = 1
LC50 : = 1.48
LC100 : = 2.2
Method : OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year : 1989
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : No further information available.
Source : Hoechst AG Frankfurt/Main
 Clariant GmbH Frankfurt am Main
 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions
 30.08.2001 (25)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type :
Species : Daphnia magna (Crustacea)
Exposure period : 24 hour(s)
Unit : mg/l
Analytical monitoring : no data
EC0 : = 1.9
EC50 : = 3.3
EC100 : = 7.4
Method : other: DIN 38412 Teil 11
Year :
GLP : no data
Test substance : no data
Source : Hoechst AG Frankfurt 80

4. Ecotoxicity

Id 105-39-5
Date 17.12.2001

Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (2) valid with restrictions
30.08.2001 (26)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type : aquatic
Species : anaerobic bact. from a domestic water treatment plant
Exposure period : 24 hour(s)
Unit : mg/l
Analytical monitoring : no
SG : 100 - 1000
Method : ETAD Fermentation tube method "Determination of damage to effluent bacteria by the Fermentation Tube Method"
Year : 1984
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : No further information available.
SG = Schaedlichkeitsgrenze

Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (2) valid with restrictions
30.08.2001 (22) (27)

Type : aquatic
Species : anaerobic bact. from a domestic water treatment plant
Exposure period : 24 hour(s)
Unit : mg/l
Analytical monitoring : no
SG : 100 - 1000
Method : ETAD Fermentation tube method "Determination of damage to effluent bacteria by the Fermentation Tube Method"
Year : 1984
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : No further information available.
SG = Schaedlichkeitsgrenze

Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (2) valid with restrictions
30.08.2001 (23) (28)

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

Species : other terrestrial plant
Endpoint : growth
Exposure period : 14 day
Unit :
Method : other: keine Daten
Year :
GLP : no data
Test substance : no data
Remark : No further information available.
 Wirkung: Gegenueber verschiedenen Pflanzenarten nach
 Bespruehung des Pflanzsubstrates mit Testloesung:
 Sprossfrischgewicht (in % der Kontrolle) nach 14taegiger
 Inkubation bei 23 +/- Grad C; FID-Analyse:

Konzentration (mg/m2)	500	1000
Weisser Senf (Sinapis alba)	125 %	120 %
Raygras (Lolium multiflorum)	83 %	96 %
Klebkraut (Galium aparine)	100 %	70 %
Mais (Zea mays)	112 %	104 %
Hafer (vermutlich Avena sativa)	104 %	90 %

Source : Hoechst AG Frankfurt 80
 Rhone-Poulenc Chimie Courbevoie Cedex
 Hoechst AG Frankfurt 80
 Hoechst AG Frankfurt/Main
 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (3) invalid
 30.08.2001 (29)

Species : other terrestrial plant
Endpoint : growth
Exposure period : 14 day
Unit :
Method : other: keine Daten
Year :
GLP : no data
Test substance : no data
Remark : Wirkung: Gegenueber verschiedenen Pflanzenarten nach
 Bespruehung des Pflanzsubstrates mit Testloesung:
 Sprossfrischgewicht (in % der Kontrolle) nach 14tagiger
 Inkubation bei 23 +/- Grad C; FID-Analyse:
 Inkubation bei 23 +/- Grad C; FID-Analyse:

Konzentration (mg/m2)	500	1000
Weisser Senf (Sinapis alba)	125 %	120 %
Raygras (Lolium multiflorum)	83 %	96 %
Klebkraut (Galium aparine)	100 %	70 %
Mais (Zea mays)	112 %	104 %
Hafer (vermutlich Avena sativa)	104 %	90 %

Source : Hoechst AG Frankfurt/Main
 Clariant GmbH Frankfurt am Main
 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (3) invalid

30.08.2001

(29)

4.6.3 TOXICITY TO OTHER NON-MAMM. TERRESTRIAL SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50	
Species	:	rat	
Strain	:	no data	
Sex	:	male	
Number of animals	:	3	
Vehicle	:	other: corn oil	
Value	:	ca. 250 mg/kg bw	
Method	:	other	
Year	:	1974	
GLP	:	no	
Test substance	:	as prescribed by 1.1 - 1.4	
Method	:	Young adult male rats were fasted overnight. They were administered the material as a solution in corn oil at a dose volume of 5 ml/kg bw at dose levels of 15.8, 31.6, 63, 126, 252, 500, and 1000 mg/kg bw. Animals were observed closely for two weeks, then submitted for pathological examination. All animals which died prior to scheduled necropsy were also submitted for pathological examination. Body weights were recorded on the day of treatment (Study Day 0), and Study Days 1, 8, and 15. Study conducted in accordance with generally accepted scientific principles. GLP not compulsory at time study was performed.	
Source	:	The Dow Chemical Company.	
Reliability	:	(2) valid with restrictions	(30)
30.08.2001			
Type	:	LD50	
Species	:	rat	
Strain	:		
Sex	:		
Number of animals	:		
Vehicle	:		
Value	:	= 180 mg/kg bw	
Method	:	other: Interne Richtlinie der Hoechst AG	
Year	:	1979	
GLP	:	no	
Test substance	:	as prescribed by 1.1 - 1.4	
Remark	:	female No further information available.	
Source	:	Hoechst AG Frankfurt 80 Rhone-Poulenc Chimie Courbevoie Cedex Hoechst AG Frankfurt 80 Hoechst AG Frankfurt/Main EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)	
Reliability	:	(2) valid with restrictions	(31)
30.08.2001			
Type	:	LD50	
Species	:	rat	
Strain	:		
Sex	:		
Number of animals	:		
Vehicle	:		
Value	:	= 50 mg/kg bw	
Method	:	other: keine Daten	
Year	:		

5. Toxicity

Id 105-39-5
Date 17.12.2001

GLP : no data
Test substance : no data
Remark : No further information available.
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions
30.08.2001 (32)

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 180 mg/kg bw
Method : other: Interne Richtlinie der Hoechst AG
Year : 1979
GLP : no
Test substance : no data
Remark : Female
No further information available.
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions
30.08.2001 (33)

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 235 mg/kg bw
Method : other: keine Angaben
Year : 1986
GLP : no data
Test substance : no data
Remark : No further information available.
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions
30.08.2001 (34)

Type : LD50
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 350 mg/kg bw
Method : other: keine Angaben
Year : 1986
GLP : no data
Test substance : no data
Remark : No further information available.

5. Toxicity

Id 105-39-5
Date 17.12.2001

Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (3) invalid
30.08.2001 (34)

5.1.2 ACUTE INHALATION TOXICITY

Type : LC50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Exposure time : 4 hour(s)
Method : other: Interne Richtlinie der Hoechst AG
Year : 1979
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : No further information available.
Wert: ca. 3.33 ml/m³
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions
30.08.2001 (35)

Type : LC50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Exposure time : 4 hour(s)
Method : other: Interne Richtlinie der Hoechst AG
Year : 1979
GLP : no
Test substance : no data
Remark : No further information available.
Result : LC50 inh. = 2 mL/h/0.6 m³ (Letalitat: 6/12 Ratten)
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions
30.08.2001 (36)

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 161 mg/kg bw
Method : other: Interne Richtlinie der Hoechst AG

5. Toxicity

Id 105-39-5
Date 17.12.2001

Year : 1979
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : Female
No further information available.
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions
30.08.2001 (37)

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 161 mg/kg bw
Method : other: Interne Richtlinie der Hoechst AG
Year : 1979
GLP : no
Test substance : no data
Remark : Female
No further information available.
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions
30.08.2001 (38)

Type : LD50
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 230 mg/kg bw
Method : other: keine Daten
Year :
GLP : no data
Test substance : no data
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions
30.08.2001 (39)

Type : LD50
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 335 mg/kg bw
Method : other: Interne Richtlinie der Hoechst AG
Year : 1979

5. Toxicity

Id 105-39-5
Date 17.12.2001

GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : No further information available.
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions
30.08.2001 (40)

Type : LD50
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 335 mg/kg bw
Method : other: Interne Richtlinie der Hoechst AG
Year : 1979
GLP : no
Test substance : no data
Remark : No further information available.
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions
30.08.2001 (41)

Type : LD50
Species : rabbit
Strain : New Zealand white
Sex : female
Number of animals :
Vehicle : other: none used
Value : = 255 mg/kg bw
Method : other
Year : 1973
GLP : no data
Test substance : other TS
Method : Female albino New Zealand White rabbits weighing approximately 5 pounds were used as the experimental animal. All rabbits were clipped as closely as possible with an Oster clipper having surgical blades and a vacuum attachment. The back of the rabbits and the sides down to about half way to the stomach area were clipped from the saddle area of the shoulders to the top of the rear leg area.
The animals were individually weighed to determine the proper dose volume. The measured volume of the liquid material was then applied undiluted to the back of the rabbit and was divided as equally as possible between the two sides of the back. If the volume was sufficiently great, the dose was kept in place by applying 8-ply gauze patches over the liquid on each side of the back. A patch of latex rubber dental dam or vinyl plastic, whichever was most compatible with the compound being tested, was then applied over the entire back area where clipped, and elastoplast tape was used to wrap the entire midsection of the rabbit to keep the gauze in place. Specially designed rabbit restraining harnesses were fitted to each rabbit at the time of treatment. These harnesses restricted

undesirable movement of the rabbits, i.e., prevented them from chewing on the taped area. The harnesses did, however, allow the rabbits complete freedom to eat and drink during the 24-hour restraining period.

The test compound remained in contact with the rabbit's skin for 24 hours. After this period of time, the gauze tape and harness were removed. The rabbits were observed for signs of toxicity or death during the 14 days immediately following dosing.

Because seven different materials were tested in this study, no data was given for the dose levels used to test each material.

Test substance : Lot No. 5635, from Matheson, Coleman, & Bell. Boiling point tested to be 142-144 degrees C.

Reliability : (2) valid with restrictions

30.08.2001

(42)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

Type : LD50
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Route of admin. : s.c.
Exposure time :
Value : = 250 - mg/kg bw
Method : other: keine Daten
Year :
GLP : no data
Test substance : no data
Source : Hoechst AG Frankfurt 80
 Rhone-Poulenc Chimie Courbevoie Cedex
 Hoechst AG Frankfurt 80
 Hoechst AG Frankfurt/Main
 Hoechst AG Frankfurt/Main
 Clariant GmbH Frankfurt am Main
 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (2) valid with restrictions

30.08.2001

(43)

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : moderately irritating
EC classification :
Method : other: Patch-Test, okklusiv
Year : 1979
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : Einwirkzeit: 24 h; 2 von 6 Tieren gestorben

5. Toxicity

Id 105-39-5
Date 17.12.2001

Source : No further information available.
: Hoechst AG Frankfurt 80
: Rhone-Poulenc Chimie Courbevoie Cedex
: Hoechst AG Frankfurt 80
: Hoechst AG Frankfurt/Main
: EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (2) valid with restrictions
30.08.2001 (44)

Species : rabbit
Concentration : 100 %
Exposure : Occlusive
Exposure time : 24 hour(s)
Number of animals : 1
PDII :
Result : moderately irritating
EC classification :
Method : other
Year :
GLP : no data
Test substance : no data
Method : A male rabbit was prepared by shaving the hair from the entire abdomen with a straight razor and barber soap. The animal was then rested for several days to allow any abrasions to heal completely and to be sure skin was suitable for use. Ten applications (unoccluded) were made to the ear over a period of 14 days. Two sites on the abdomen were used for applications: one intact, the other cross-hatched with a sharp hypodermic needle to penetrate the stratum corneum but not to produce more than a trace of bleeding. Ten applications were made to the intact abdominal site over a period of 14 days. Three consecutive daily applications were made to the abraded site. Both abdominal sites were covered with 1X1 cotton pads and held place with a single cotton cloth taped to remaining body hair. Applications were discontinued upon production of a substantial skin burn, or if the animal died.

Result : The test was discontinued after 6 applications to the ear and intact abdomen, when it was found dead. Three applications to the abraded abdomen had also been completed.

Reliability : (2) valid with restrictions
30.08.2001 (30)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : irritating
EC classification : irritating
Method : OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year : 1988
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : Einwirkzeit: 4 h
: No further information available.

Source : Hoechst AG Frankfurt 80
: Rhone-Poulenc Chimie Courbevoie Cedex
: Hoechst AG Frankfurt 80
: Hoechst AG Frankfurt/Main
: EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

5. Toxicity

Id 105-39-5
Date 17.12.2001

Reliability : (2) valid with restrictions
30.08.2001 (45)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : moderately irritating
EC classification :
Method : other: Patch-Test, okklusiv
Year : 1979
GLP : no
Test substance : no data
Remark : Einwirkzeit: 24 h
No further information available.
Result : Letalitat: 2/6 Kaninchen
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (2) valid with restrictions
30.08.2001 (46)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : irritating
EC classification : irritating
Method : OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year : 1988
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : Einwirkzeit: 4 h
No further information available.
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (2) valid with restrictions
30.08.2001 (47)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : moderately irritating
EC classification :
Method : other: keine Angaben
Year : 1979
GLP : no
Test substance : no data
Remark : No further information available.
Patch-Test, Einwirkzeit 24 Stunden, 100 mg/kg KG
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions

5. Toxicity

Id 105-39-5
Date 17.12.2001

30.08.2001 (48)

Species : rabbit
Concentration : 100 %
Exposure : Occlusive
Exposure time : 4 hour(s)
Number of animals : 6
PDII :
Result : moderately irritating
EC classification :
Method : other
Year : 1972
GLP : no data
Test substance : no data
Method : Six New Zealand White female rabbits were prepared by clipping the hair from an area approximately 4 x 4 in. in size on the back with electric clippers 24 hours before application of the material to be evaluated. The rabbits were restrained in a stock, and the material was applied under a 1 x 1 in. gauze pad held in place with adhesive tape to two sites, one abraded and one intact. For the abraded site, the skin was cross-hatched with a hypodermic needle so as to penetrate the stratum corneum but not to produce more than a trace of bleeding. Each rabbit was loosely covered with a plastic cuff. AT the end of four hours, the gauze patches were removed and the application sites graded for erythema, edema, and necrosis. The application sites were washed with soap and water and held for additional readings at 24 and 48 hours, if necessary.
Source : The Dow Chemical Company
Reliability : (2) valid with restrictions

30.08.2001 (49)

Species : human
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result :
EC classification :
Method : other: Patch-Test
Year :
GLP : no data
Test substance : no data
Remark : Positive Reaktion bei einem Patienten
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions

30.08.2001 (50)

5.2.2 EYE IRRITATION

Species : rabbit
Concentration : undiluted
Dose : 2 other: drops
Exposure Time : unspecified

5. Toxicity

Id 105-39-5
Date 17.12.2001

Comment :
Number of animals : 1
Result : highly irritating
EC classification :
Method : other
Year : 1973
GLP : no data
Test substance : no data
Method : Both eyes of a male New Zealand White rabbit were stained with 5% fluorescein dye and examined for evidence of injury or alterations. The rabbit was then allowed to rest for 24 hours before test.

Two drops of the material were introduced into the right eye. The eye was washed within 30 seconds for 2 minutes in a flowing stream of tepid water. Two drops of material were introduced in a similar fashion to the left eye, but this eye was left unwashed.

Immediately after instillation into each eye, the rabbit was examined for signs of discomfort. Within 2-3 minutes after the unwashed eye was treated, each eye was observed for conjunctival and corneal response. Similar observations were made on both eyes at 1 hour, 24 hours, 48 hours, and 6-8 days post-treatment. Examinations were conducted both with and without fluorescein dye.

Result : Rabbit had very severe conjunctival irritation and moderate corneal and iridal effects in the unwashed eye after 48 hours, while the washed eye appeared normal. The test was terminated after 7 days, when the unwashed eye still had significant conjunctival irritation and moderate corneal and slight iridal effects.

Reliability : (2) valid with restrictions
30.08.2001 (30)

Species : rabbit
Concentration :
Dose :
Exposure Time :
Comment :
Number of animals :
Result : highly irritating
EC classification : risk of serious damage to eyes
Method : other: Interne Richtlinie der Hoechst AG
Year : 1979
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : Einwirkzeit: 24 h
No further information available.

Source : Hoechst AG Frankfurt 80
Rhône-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (2) valid with restrictions
30.08.2001 (44)

Species : rabbit
Concentration :
Dose :
Exposure Time :
Comment :

5. Toxicity

Id 105-39-5
Date 17.12.2001

Number of animals :
Result : highly corrosive
EC classification :
Method : other: keine Daten
Year :
GLP : no data
Test substance : no data
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions
30.08.2001 (51)

Species : rabbit
Concentration :
Dose :
Exposure Time :
Comment :
Number of animals :
Result : highly irritating
EC classification : risk of serious damage to eyes
Method : other: Interne Richtlinie der Hoechst AG
Year : 1979
GLP : no
Test substance : no data
Remark : Einwirkzeit: 24 h
No further information available.
Result : R41
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions
30.08.2001 (46)

Species : rabbit
Concentration :
Dose :
Exposure Time :
Comment :
Number of animals :
Result : highly irritating
EC classification :
Method : other: keine Daten
Year :
GLP : no data
Test substance : no data
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions
30.08.2001 (51)

Species : human
Concentration :
Dose :
Exposure Time :
Comment :
Number of animals :
Result : highly corrosive
EC classification :

5. Toxicity

Id 105-39-5
Date 17.12.2001

Method : other: keine Daten
Year :
GLP : no data
Test substance : no data
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions
30.08.2001 (51)

5.3 SENSITIZATION

Type : Guinea pig maximization test
Species : guinea pig
Number of animals :
Vehicle :
Result : not sensitizing
Classification :
Method : other: keine Daten
Year :
GLP : no data
Test substance : no data
Remark : 5/20 Tiere = 25 % zeigten eine positive Reaktion
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (1) valid without restriction
30.08.2001 (50)

Type : Guinea pig maximization test
Species : guinea pig
Number of animals :
Vehicle :
Result : sensitizing
Classification :
Method : other: keine Daten
Year :
GLP : no data
Test substance : no data
Remark : 20/20 Tiere zeigten eine positive Reaktion
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (1) valid without restriction
30.08.2001 (52)

Type : Guinea pig maximization test
Species : guinea pig
Number of animals :
Vehicle :
Result : sensitizing
Classification :
Method : other: keine Daten
Year :

5. Toxicity

Id 105-39-5
Date 17.12.2001

GLP : no data
Test substance : no data
Remark : 15/19 Tiere zeigten eine positive Reaktion
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (1) valid without restriction
30.08.2001 (53)

Type : Guinea pig maximization test
Species : guinea pig
Number of animals :
Vehicle :
Result : sensitizing
Classification :
Method : other: keine Daten
Year :
GLP : no data
Test substance : no data
Remark : 15/19 Tiere zeigten eine positive Reaktion
Source : Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (1) valid without restriction
30.08.2001 (53)

Type : Guinea pig maximization test
Species : guinea pig
Number of animals :
Vehicle :
Result : not sensitizing
Classification :
Method : other: keine Daten
Year :
GLP : no data
Test substance : no data
Remark : 5/20 Tiere = 25 % zeigten eine positive Reaktion
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : 5 % Chloressigsaeureethylester in 50 % Ethanol
Reliability : (2) valid with restrictions
30.08.2001 (50)

Type : Guinea pig maximization test
Species : guinea pig
Number of animals :
Vehicle :
Result : sensitizing
Classification :
Method : other: keine Daten
Year :
GLP : no data
Test substance : no data
Remark : 20/20 Tiere zeigten eine positive Reaktion
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : 80% Monochloressigsaeure in 50 % Ethanol
Reliability : (1) valid without restriction
30.08.2001 (52)

5. Toxicity

Id 105-39-5
Date 17.12.2001

Type : Guinea pig maximization test
Species : guinea pig
Number of animals :
Vehicle :
Result : sensitizing
Classification :
Method : other: keine Daten
Year :
GLP : no data
Test substance : no data
Remark : 15/19 Tiere zeigten eine positive Reaktion
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : 5 % Chloressigsäureethylester in 50 % Ethanol
Reliability : (1) valid without restriction
30.08.2001 (53)

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test
System of testing : Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration :
Cytotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471 "Genetic Toxicology: Salmonella typhimurium Reverse Mutation Assay"
Year : 1983
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : No further information available.
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (1) valid without restriction
30.08.2001 (54)

Type : Ames test
System of testing : Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration :
Cytotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471 "Genetic Toxicology: Salmonella typhimurium Reverse Mutation Assay"
Year : 1992
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : No further information available.
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main

5. Toxicity

Id 105-39-5
Date 17.12.2001

Reliability : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
30.08.2001 : (1) valid without restriction (55)

Type : Ames test
System of testing : Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration :
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year : 1983
GLP : no
Test substance : no data
Remark : No further information available.
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main

Reliability : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
30.08.2001 : (2) valid with restrictions (56)

Type : Ames test
System of testing : Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration :
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year : 1992
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main

Reliability : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
30.08.2001 : (1) valid without restriction (55)

Type : Ames test
System of testing : Escherichia coli WP2uvrA
Concentration :
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 472 "Genetic Toxicology: Escherichia coli Reverse Mutation Assay"
Year : 1983
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Source : Hoechst AG Frankfurt 80
Rhône-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main

Reliability : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
30.08.2001 : (1) valid without restriction (54)

Type : Ames test
System of testing : Escherichia coli WP2uvrA
Concentration :
Cycotoxic conc. :

5. Toxicity

Id 105-39-5
Date 17.12.2001

Metabolic activation Result Method	: with and without : negative : OECD Guide-line 472 "Genetic Toxicology: Escherichia coli Reverse Mutation Assay"
Year	: 1983
GLP	: no
Test substance	: no data
Remark	: No further information available.
Source	: Hoechst AG Frankfurt/Main Clariant GmbH Frankfurt am Main EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability 30.08.2001	: (2) valid with restrictions (56)
Type	: Ames test
System of testing	: Salmonella typh. TA102, TA2638, E. coli WP2/pKM101 und WP2uvrA/pK101
Concentration	: 0, 78, 156, 313, 500, 625, 1000, 1250, 1500, 2000, 2500, 5000 ug/plate
Cycotoxic conc.	: TA102: 1500; TA2638: 1500; none noted for others
Metabolic activation Result	: with and without : negative
Method	: other: keine Angaben
Year	: 1996
GLP	: no data
Test substance	: no data
Method	: Plate incorporation method with or without metabolic activation, essentially as described by Maron and Ames, 1983 (Mutation Research 113: 173-215). Positive controls were included in each experiment. The results were analyzed for statistical significance using a linear regression test recommended by UKEMS and carried out at the 1% significance level. Doses with observed cytotoxicity, which was judged by a toxicity to the background lawn and/or a reduction in the number of revertent colonies, were excluded from the statistical analysis.
Remark	: No further information available.
Result	: in der Publikation wird von einem von zwei Prufinstituten mit E. coli WP2uvrA/pKM101 ein positives Ergebnis angegeben, die Revertanzahl ist jedoch nicht um das doppelte erhöht.
Source	: Hoechst AG Frankfurt/Main Clariant GmbH Frankfurt am Main EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability 30.08.2001	: (2) valid with restrictions (57)
Type	: Ames test
System of testing	: Salmonella typhimurium TA 100
Concentration	:
Cycotoxic conc.	:
Metabolic activation Result	: with and without : negative
Method	: other: keine Daten
Year	:
GLP	: no data
Test substance	: no data
Remark	: No further information available.
Source	: Hoechst AG Frankfurt 80 Rhone-Poulenc Chimie Courbevoie Cedex Hoechst AG Frankfurt 80 Hoechst AG Frankfurt/Main Hoechst AG Frankfurt/Main Clariant GmbH Frankfurt am Main

5. Toxicity

Id 105-39-5
Date 17.12.2001

Reliability : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
30.08.2001 : (2) valid with restrictions (58)

Type : other: Genmutationstest
System of testing : Saccharomyces cerevisiae D7 bzw. XV185-14C
Concentration : Not specified
Cycotoxic conc. : Not specified
Metabolic activation : with and without
Result : negative
Method : other: keine Daten
Year : 1985
GLP : no data
Test substance : other TS
Method : Yeast strains D7 and XV185-14C were used for testing according to the method described by Von Borstel et al. (1981; Short-Term Tests for Chemical Carcinogens, Springer, NY, pp. 171-174) using exponential phase cultures for Trp+ gene convertants or for reversion of the histidine, homoserine, and tryptophan markers, respectively.

Remark : No further information available.
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Test substance : Research grade material from Pfaltz and Bauer.
Reliability : (2) valid with restrictions (59)
30.08.2001

5.6 GENETIC TOXICITY 'IN VITRO'

5.7 CARCINOGENITY

Species : mouse
Sex : female
Strain : other: ICR/Ha Swiss
Route of admin. : dermal
Exposure period : 580 Day
Frequency of treatment : 3 applications/week
Post. obs. period :
Doses : 0.2 mg/0.1 ml Acetone
Result : negative
Control group : yes, concurrent vehicle
Method : other: keine Daten
Year :
GLP : no data
Test substance : no data
Remark : 50 mice/test group
Result : Nach der Applikation (durchschnittliche Ueberlebensdauer 552 Tage) keine Tumoren.
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main

5. Toxicity

Id 105-39-5
Date 17.12.2001

EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
The Dow Chemical Company

Reliability : (2) valid with restrictions (60)
30.08.2001

Species : mouse
Sex : female
Strain : other: ICR/Ha Swiss
Route of admin. : dermal
Exposure period : 580 Tage
Frequency of treatment : 3mal/Woche
Post. obs. period :
Doses : 0, 2 mg/0.1 ml Aceton
Result :
Control group : yes, concurrent vehicle
Method : other: keine Daten
Year :
GLP : no data
Test substance : no data
Remark : 50 Tiere/Gruppe
Result : Nach der Applikation (durchschnittliche Überlebensdauer 552 Tage) keine Tumoren.

Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main

EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (2) valid with restrictions (60)
30.08.2001

Species : mouse
Sex : male/female
Strain : other: A/St
Route of admin. : i.p.
Exposure period : 8 Wochen
Frequency of treatment : 3mal/Woche
Post. obs. period : 24 Wochen nach der ersten Applikation
Doses : 0, 0.25, 0.5, 1.0 mM/kg Kgw.
Result :
Control group : yes
Method : other: keine Daten
Year :
GLP : no data
Test substance : no data
Remark : 10 Tiere/Geschlecht/Gruppe
Result : In der hoechsten Dosisgruppe in einem von zwei statistischen Tests signifikant erhoehte Inzidenz an Lungentumoren (0.6 Tumoren/Tier; Kontrolle: 0.19 Tumoren/Tier); Relevanz der Befunde aufgrund methodischer Maengel fraglich.

Source : Hoechst AG Frankfurt 80
Rhône-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main

EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (2) valid with restrictions (61)
30.08.2001

Species : mouse
Sex : male/female
Strain : other: A/St
Route of admin. : i.p.
Exposure period : 8 Wochen

5. Toxicity

Id 105-39-5
Date 17.12.2001

Frequency of treatment : 3mal/Woche
Post. obs. period : 24 Wochen nach der ersten Applikation
Doses : 0, 0.25, 0.5, 1.0 mM/kg Kgw.
Result :
Control group : yes
Method : other: keine Daten
Year :
GLP : no data
Test substance : no data
Remark : 10 Tiere/Geschlecht/Gruppe
No further information available.
Result : In der höchsten Dosisgruppe in einem von zwei statistischen Tests signifikant erhöhte Inzidenz an Lungentumoren (0.6 Tumoren/Tier; Kontrolle: 0.19 Tumoren/Tier); Relevanz der Befunde aufgrund methodischer Mängel fraglich.
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions
30.08.2001 (61)

Species : mouse
Sex : female
Strain : other: ICR/Ha Swiss
Route of admin. : s.c.
Exposure period : 580 Tage
Frequency of treatment : 1mal/Woche
Post. obs. period :
Doses : 1 mg/0.05 ml Tricaprylin
Result :
Control group : yes, concurrent vehicle
Method : other: keine Daten
Year :
GLP : no data
Test substance : no data
Remark : 50 Tiere/Gruppe
Result : Nach der Applikation (durchschnittliche Ueberlebensdauer 471 Tage) trat bei einem Tier ein lokales Sarkom auf.
Source : Hoechst AG Frankfurt 80
Rhône-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions
30.08.2001 (60)

Species : mouse
Sex : female
Strain : other: ICR/Ha Swiss
Route of admin. : s.c.
Exposure period : 580 Tage
Frequency of treatment : 1mal/Woche
Post. obs. period :
Doses : 1 mg/0.05 ml Tricaprylin
Result :
Control group : yes, concurrent vehicle
Method : other: keine Daten
Year :
GLP : no data

5. Toxicity

Id 105-39-5
Date 17.12.2001

Test substance : no data
Remark : 50 Tiere/Gruppe
Result : Nach der Applikation (durchschnittliche Überlebensdauer 471 Tage) trat bei einem Tier ein lokales Sarkom auf.
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions
30.08.2001 (60)

5.8 TOXICITY TO REPRODUCTION

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.10 OTHER RELEVANT INFORMATION

Type : other
Remark : Durch Hydrolyse von Chloressigsaeureethylester entsteht Monochloressigsaeure. Auch bei dieser Verbindung haben sich in Kanzerogenitaetsstudien nach dermalen und subkutaner Applikation an der Maus sowie nach oraler Applikation (Schlundsondierung) an Maus und Ratte keine Hinweise auf eine kanzerogene Wirkung ergeben.
Source : Hoechst AG Frankfurt 80
Rhone-Poulenc Chimie Courbevoie Cedex
Hoechst AG Frankfurt 80
Hoechst AG Frankfurt/Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (4) not assignable
30.08.2001

Type : other
Remark : Durch Hydrolyse von Chloressigsaeureethylester entsteht Monochloressigsaeure. Auch bei dieser Verbindung haben sich in Kanzerogenitatsstudien nach dermalen und subkutaner Applikation an der Maus sowie nach oraler Applikation (Schlundsondierung) an Maus und Ratte keine Hinweise auf eine kanzerogene Wirkung ergeben.
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (4) not assignable
30.08.2001

Type : other
Remark : Tierversuche haben ergeben, da? Benetzung von nur 3 % der Hautoberflache todlich wirken kann.
Source : Hoechst AG Frankfurt/Main
Clariant GmbH Frankfurt am Main
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (4) not assignable
30.08.2001 (62)

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