Benzotriazoles Coalition

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December 31, 2001

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

Attn: Chemical Right-to-Know Program; HPV Reference Number: [redacted]

Dear Administrator Whitman:

The Benzotriazoles Coalition was formed under the management of SOCMA's Association Management Center to volunteer as a sponsor in the HPV Challenge. For 2001, the Coalition committed to gathering existing data and making it publicly available, identifying potential data needs and preparing a test plan to reflect those findings. The Coalition has fulfilled this portion of the commitment and is including those materials in this package.

As you will note, the Coalition's test plan has identified the need for a developmental toxicity test for one of the materials, which can then be used as a surrogate for the others. The Coalition would like to carry out the work proposed in the test plan, but assistance will be needed by the Agency to achieve these objectives.

According to Department of Commerce statistics, in the past year the benzotriazoles markets have experienced extraordinary competition from overseas, China in particular. Prices for tolyltriazole dropped by approximately ten percent from 2000 to 2001. Prices for benzotriazole have dropped as well. Imports have more than doubled in that same period. In fact, China has 60 percent of worldwide production capacity for benzotriazoles. If the Coalition continues with its test plan, the member companies will be placed at a further competitive disadvantage in the marketplace.

The Coalition has repeatedly approached importers and requested that they join our efforts, but they have expressed no intent of doing so. After much consideration, the Coalition has reasoned that the most fair, practical way to move forward and fulfill its entire commitment under the HPV Challenge, is through regulatory action, such as a rulemaking under TSCA Section 4.

The Benzotriazoles Coalition supports EPA's efforts to work with industry under voluntary agreements to provide important health and environmental information to the public. The Coalition especially supports the HPV Challenge and is serious about fulfilling its commitment. As you can see in the test plan and robust summaries, a great deal of work has already been done in this regard. With the Agency's assistance, by including the benzotriazoles category in a rule-making, our commitment can be fulfilled, while maintaining fairness and equity among all players in the marketplace. If you or your staff have any questions, please feel free to contact me.

Sincerely,
James Cooper
Executive Director

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Benzotriazoles
Category Justification and Testing Rationale

CAS Nos. 95-14-7, 29385-43-1 and 64665-57-2

Benzotriazoles Coalition
Synthetic Organic Chemical Manufacturers Association

December, 2001

List of Member Companies in the Benzotriazoles Coalition

The Benzotriazoles Coalition of the Synthetic Organic Chemical Manufacturers Association (SOCMA) includes the following member companies: Bayer Corporation and PMC Specialties Group, Inc.

Executive Summary

The Benzotriazoles Coalition, and its member companies, hereby submit for review and public comment their test plan for the Benzotriazoles category of chemicals under the Environmental Protection Agency's (EPA) High Production Volume (HPV) Chemical Challenge Program.

As discussed in the report that follows, Benzotriazole chemicals are used primarily as chemical intermediates, copper corrosion inhibitors, used in ultra-violet stabilization applications, photographic applications, and as ingredients of de-icing fluids for airplanes.

Relying on several factors specified in EPA's guidance document on "Development of Chemical Categories in the HPV Challenge Program," in which use of chemical categories is encouraged, the following closely related chemicals constitute a chemical category:

1-H-benzotriazole	(95-14-7)
1-H-benzotriazole, 4 (or 5) methyl	(29385-43-1)
1-H-benzotriazole, 4 (or 5) methyl, sodium salt	(64665-57-2)

Benzotriazole is the parent chemical in this category with the others having a methyl substituent at position 4 or 5. The Sodium salt will dissociate to the methyl benzotriazole in aqueous solution.

Existing data for members of this category indicate that they are of low concern for aquatic and mammalian toxicity, will partition to soil and water and are readily biodegradable. We conclude that there is sufficient data on the members of this, except for the endpoint of Developmental Toxicity. Therefore, to meet requirements of the HPV Chemical Challenge Program, a Teratogenicity Study (OECD 414) on benzotriazole is proposed.

The Benzotriazoles Coalition would like to carry out the work proposed in the test plan, but assistance will be needed by the Agency to achieve these objectives. Extraordinary competition from overseas has placed US companies in a competitive disadvantage in the marketplace.

The Coalition has repeatedly approached importers and requested that they join our efforts, but they have expressed no intent of doing so. After much consideration, the Coalition has reasoned that the most fair, practical way to move forward and fulfill its entire commitment under the HPV Challenge, is through regulatory action, such as a rulemaking under TSCA Section 4.

Introduction

A provision for the use of categories to reduce testing needs is included under EPA's HPV Program. Specifically, categories may be formed based on structural similarity, through analogy, or through a combination of category and analogy for use with single chemicals. The benefits of using a category approach are numerous and include: accelerated release of hazard information to the public; reduction in the number of animals used for testing; and an economic savings as a result of a reduced testing program.

The Benzotriazoles that form this category based on structural similarity, arranged in order of increasing molecular weight, are:

1-H-benzotriazole	(95-14-7)
1-H-benzotriazole, methyl	(29385-43-1)
1-H-benzotriazole, methyl, sodium salt	(64665-57-2)

Development of the Benzotriazoles category

EPA has described a stepwise process for developing categories. These steps include:

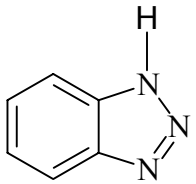
- Grouping a series of like chemicals, including the definition of criteria for the group.
- Gathering data on physicochemical properties, environmental fate and effects, and health effects for each member of the category.
- Evaluating the data for adequacy.
- Constructing a matrix of available and unavailable data.
- Determining whether there is a correlation among category members and data gathered.

Definition of the Benzotriazoles category

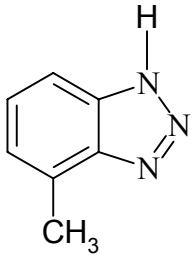
As defined by EPA under the HPV Program, a chemical category is "a group of chemicals whose physicochemical and toxicological properties are likely to be similar or follow a regular pattern as a result of structural similarity." The similarities should be based on a common functional group, common precursors or breakdown products (resulting in structurally similar chemicals) and an incremental and constant change across the category. The goal of developing a chemical category is to use interpolation and/or extrapolation to assess chemicals rather than conducting additional testing.

Structural Similarity.

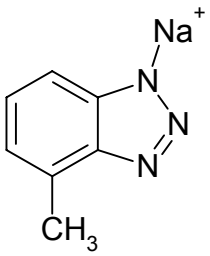
A key factor supporting the classification of these chemicals as a category is their structural similarity. The chemicals within the Benzotriazoles category are defined as illustrated below.



1-H-Benzotriazole
(CAS# 95-14-7)



1-H-Benzotriazole, 4 (or 5)-methyl
(CAS# 29385-43-1)



1-H-Benzotriazole, 4 (or 5)-methyl, sodium salt
(CAS# 64665-57-2)

Figure 1. Chemical Structures

Matrix of SIDS Endpoints

In order to construct a matrix of SIDS endpoints for the members of the Benzotriazoles category, the data on physicochemical properties, environmental fate, ecotoxicity and health effects for each member of the category was collected and evaluated for adequacy. The results of these activities are presented in the tables and text below, as well as the attached IUCLID documents, providing a matrix of available data.

Correlation of Physicochemical Properties

The physicochemical properties of the members of the Benzotriazoles category are presented in **Table 1**. The Benzotriazoles are non-flammable, colorless or pale colored solids with low vapor pressure and low partition coefficients. The similarities in the other physicochemical properties of these chemicals are explained by similarities in their chemical structure, and provide justification of this group of chemicals as a category within the HPV Challenge Program.

All members of the category have measured or calculated data on physicochemical properties. There are no data gaps; no additional testing is needed to meet requirements of the HPV Chemical Challenge Program.

Correlation of Environmental Fate

The HPV Challenge Program requires that hydrolysis, photodegradation, biodegradation and environmental transport information be presented for each chemical or bridged to each member of a category. The EPIWIN modeling Program was used to calculate the photodegradation and fugacity for each chemical in the category. The members of this category have photodegradation half-lives of 3-10 days.

Adequate biodegradation data exist for all chemicals in this category. All are categorized as "readily biodegradable" with degradation rates ≥70% after 28 days.

Partitioning to soil and water fractions (vs. air and sediment) is expected according to Fugacity Level III calculations. Default "input values" of 1000 kg/hr were used for the modeling.

Hydrolysis data on benzotriazole demonstrates that it is a weak acid and somewhat soluble in water. The pKa for this reaction is 8.2 (Boyer, 1961). The reaction suggests that benzotriazole will be less soluble in pH <7 (such as rainwater) and more soluble in solutions >7 (such as seawater) than in distilled water. Benzotriazole reacts with solutions of alkali metal hydroxides producing soluble alkali salts (NTIS PB-266 366, 1977). Sodium tolyltriazole is sold as aqueous solution; it is stable in water, it does not hydrolyze.

Data is available or bridged for all Environmental Fate endpoints for this category (See **Table 2**). No additional testing is needed to meet requirements of the HPV Chemical Challenge Program.

Correlation of Ecotoxicity

The HPV Challenge Program requires that an acute aquatic toxicity test in fish, invertebrates, and algae be performed or bridged to each member of a category. Existing data indicate that the members of the Benzo and tolyl triazoles have low toxicity to fish (LC_{50} = 21 - >175 mg/l), Daphnia (EC_{50} = 35-280 mg/l), and algae (EC_{50} = 26-231 mg/l).

No additional aquatic toxicity tests are proposed for this category as it has been adequately characterized for purposes of the HPV Chemical Challenge Program.

Correlation of Health Effects

Acute Mammalian Toxicity

Acute oral, dermal and inhalation toxicity data for the category is summarized in **Table 4**. All chemicals have test data, all show moderate toxicity following oral administration and low toxicity following dermal administration.

Dose response studies by the oral route, conducted by Sherwin-Williams Company in 1976, show that benzotriazole is slightly more toxic than tolyltriazole and since the slopes of both dose response curves are similar it was predicted that mechanism of action is similar for both chemicals (NTIS PB-266 366, 1977). Investigations of dermal toxicity at 2000 mg/kg in rabbits resulted in essentially identical results for the benzo- and tolyl-triazole (NTIS PB-266 366, 1977).

The similarity in the order of toxicity for these chemicals is consistent with their similar chemical structure and physicochemical properties and supports the scientific justification of these chemicals as a category within the HPV Challenge Program.

The HPV Challenge Program requires that either an acute test be performed or bridged to each member of a category. Adequate acute oral and dermal toxicity tests exist for all members of the category and inhalation testing has been conducted on two of the chemicals. The acute toxicity of the category has been adequately evaluated with respect to acute toxicity endpoints, and no additional acute toxicity testing is proposed for purposes of the HPV Challenge Program**.**

Repeat Dose Toxicity

A summary of the repeat dose toxicity data for the Benzotriazoles category is presented in **Table 4**.

Repeat dose studies (28 d or 18-24 month studies) have been conducted with two of the Benzotriazoles and demonstrate an apparent reduction in toxicity with increasing molecular weight. The repeat dose toxicity of the sodium salt (CAS#64665-57-2) is expected to be similar to the repeat dose toxicity of tolyl triazole (29385-43-1), since the sodium salt will dissociate to the methyl benzotriazole in aqueous solution.

By bridging existing data to the one chemical where no data was found, the repeat dose aspect of the category has been evaluated adequately, and no additional testing is proposed to meet requirements of the HPV Challenge Program**.**

Mutagenicity

A summary of the mutagenicity information for the Benzotriazole category is presented in **Table 4**. The weight of evidence for the members of this category indicates these chemicals are not mutagenic or clastogenic. By bridging existing data to the sodium salt, which will dissociate to the methyl benzotriazole in aqueous solution, the mutagenicity aspect of the category has been evaluated adequately, and no additional testing is proposed to meet requirements of the HPV Challenge Program**.**

Reproductive and Developmental Toxicity.

Consideration was given to effects on reproductive organs in repeated exposure studies to determine whether reproductive toxicity studies were needed. The 78 week oral study of 1H-benzotriazole in Fischer 344 rats did not find any evidence of pathology in the reproductive organs. The 104 week oral study of 1H-benzotriazole in B6C3F1 mice did not find any evidence of pathology in the reproductive organs. The reproductive organs examined were: prostate/testis/epididymis of males and uterus/ovaries of females. These chemicals are covered by the chronic data discussed to meet requirements of the HPV Challenge Program and no further testing for reproductive toxicity is proposed.

No data was found on the Developmental toxicity of benzo- and tolyl- triazole.
Therefore, to meet requirements of the HPV Chemical Challenge Program, a Teratogenicity Study (OECD 414) on benzotriazole is proposed. Benzotriazole was chosen because it is slightly more toxic than tolyltriazole and will provide the worst case scenario.

Conclusion.

In consideration of animal welfare concerns to minimize the use of animals in the testing of chemicals, the Panel has conducted a thorough literature search for all available data, published and unpublished. It has performed an analysis of the adequacy of the existing data. Further, it developed a scientifically supportable category of related chemicals and used structure-activity relationship information to fill certain data gaps. The use of animals in this proposed test plan has been minimized.

Based upon the data provided in this report and the attached IUCLID documents, the physicochemical and toxicological properties of the Benzotriazoles category members are similar and follow a regular pattern as a result of that structural similarity. Therefore, the EPA definition of a chemical category has been met.

Summary Endpoint Matrix / Test Plan

All endpoints of the category has been adequately characterized, except for Developmental Toxicity, therefore to fulfill requirements of the HPV Chemical Challenge Program, a Teratogenicity Study (OECD 414) on benzotriazole is proposed.
The summary endpoint matrix is included as **Table 5** of this document.

Background Information: Manufacturing and Commercial Applications

Manufacturing

Triazoles (Benzo and Tolyl) are produced by the reaction of unsubstituted and substituted aromatic amines with other nitrogen donors. The formed product(s) are further purified before distribution to the market place.

Commercial Applications

Benzotriazoles are used primarily as chemical intermediates, copper corrosion inhibitors, in ultra-violet stabilization applications, photographic applications, and as ingredients of de-icing fluids for airplanes.

Shipping/Distribution

Triazoles (Benzo and Tolyl) are shipped throughout the world from Manufacturing plants.

Worker/Consumer Exposure

The Benzotriazoles industry has a long safety record in handling these chemicals by both the manufacturers and users. Exposure of workers handling the Benzotriazole materials is likely to be highest in the area of packaging. These materials are powders or liquids of very low vapor pressure, thus during the packaging process there is a low potential for inhalation exposure except as nuisance dust. Depending on handling procedures and filling equipment, dermal contact to the liquid is also possible.

Table 1. Matrix of Available and Adequate Data on the Benzotriazoles Category Physico-chemical Properties

Chemical **CAS#**	**1-H-Benzotriazole** **95-14-7**	**1-H-Benzotriazole, 4 (or 5)-methyl** **29385-43-1**	**1-H-Benzotriazole, 4 (or 5)-methyl, sodium salt** **64665-57-2**
Molecular Weight:	119.1	133.2	155
Physical State	Yellow solid or powder	Beige granules	Clear yellow to amber liquid
MeltingPoint	100ºC	76-87ºC	-5 to -10ºC
Boiling Point	204ºC @ 20 hPa	160ºC @ 2.67hPa	~ 106ºC @ 1013 hPa
Relative Density	1.19 g/cm^3 @ 100ºC	1.13 g/cm^3 @ 100ºC	1.18 g/cm^3 @ 20ºc
Vapor Pressure	0.000797 hPa @ 25ºC (EPIWIN)	0.00001 hPa @ 25ºC 0.000797 hPa @ 25ºC (EPIWIN)	.0533 hPa @ 20ºC < 0.00001 hPa @ 25ºC (EPIWIN)
PartitionCoefficient ($logP_{ow}$)	1.34	1.71	0.658
Water Solubility	1-5 mg/l @24ºC	<0.1g/l @18ºC	55 vol % @20ºC

EPIWIN = EPIWIN modeling Program. Meylan, W. and Howard, P. (1999)

Table 2. Matrix of Available and Adequate Data on the Benzotriazoles category Environmental Fate

Endpoint	**1-H-Benzotriazole** **95-14-7**	**1-H-Benzotriazole, 4 (or 5)-methyl** **29385-43-1**	**1-H-Benzotriazole, 4 (or 5)-methyl, sodium salt** **64665-57-2**
Photodegradation T ½ =	10.7 days (AOP)	3.9 days (AOP)	3.1 days (AOP)
Hydrolysis	pKa = 8.2	No data found	Stable. Sodium tolyltriazole dissolves in water, it does not hydrolyze. Sold as aqueous solution
Biodegradation	90% after 28 D	77% after 28 D	70% after 28 D
Fugacity Level III			
Air (%)	4.6	2.8	<0.001
Water (%)	42.3	39.3	43.5
Soil (%)	53.1	57.8	56.4
Sediment (%)	0.0869	0.0934	0.0754

AOP = AOP Program, version 1.89. EPIWIN modeling Program. Meylan, W. and Howard, P. (1999)

Table 3. Matrix of Available and Adequate Data on the Benzotriazoles category Ecotoxicity

Endpoint	**1-H-Benzotriazole** **95-14-7**	**1-H-Benzotriazole, 4 (or 5)-methyl** **29385-43-1**	**1-H-Benzotriazole, 4 (or 5)-methyl, sodium salt** **64665-57-2**
Acute Fish Toxicity 96 hr LC50	*B. rerio* = **>100 mg/l** *S. gairdneri* = **39 mg/l**	*B. rerio* = **65 mg/l** *L. macrochirus* = **31 mg/l** *P. promelas* = **25.5 mg/l** *S. gairdneri* = **21.4 mg/l**	*L. macrochirus* = **>173 mg/l** *S. gairdneri* = **~ 25 mg/l** *B. rerio* = **122 mg/l**
Acute Invertebrate Toxicity 48 hr EC50	*D. magna* = **91 - 141 mg/l**	*D. magna* = **35.4 mg/l**	*D. magna* LC50 = **280 mg/l**
Algal Toxicity 72 hr EC50	*S. subspicatus* = **231 mg/l** (growth) **102 mg/l** (biomass)	*S. subspicatus* = **62 mg/l** (growth) **32 mg/l** (biomass)	*S. capricornutum* = **26.2 mg/l** (growth) **32 mg/l** (biomass) (96 hr)

Table 4. Matrix of Available and Adequate Data on the Benzotriazoles category
Mammalian Toxicity

Endpoint	**1-H-Benzotriazole** **95-14-7**	**1-H-Benzotriazole, 4 (or 5)-methyl** **29385-43-1**	**1-H-Benzotriazole, 4 (or 5)-methyl, sodium salt** **64665-57-2**
Acute Toxicity			
Oral LD50	**560-909 mg/kg bw** (rat)	**1470 - 1830 mg/kg bw** (rat)	**640-1980mg/kg bw** (rat) **mg/kg bw** (rabbit)
Dermal LD50	**> 10,000 mg/kg bw** (rabbit)	**> 4,000 mg/kg bw** (rabbit)	**> 2,000 mg/kg bw** (rabbit)
Inhalation LC50	**> 1.5 mg/l** (4 hr) (rat)	**> 1.73 mg/l** (1 hr) (rat)	No data found
Repeated Dose NOAEL=	**12.100 ppm** (oral - rat –18 mos) **23,500 ppm** (oral - mouse –24 mos)	150 mg/kg bw (oral- rat - 29 D)	No data found
Mutagenicity – gene mutation	Ames – positive HGPRT - negative	Ames – negative	No data found
Mutagenicity – chromosome aberration	Micronucleus test (mouse) - negative	DNA Damage and Repair – negative Micronucleus test (mouse) - negative	No data found
Reproductive Toxicity	No pathology of reproductive organs **12.100 ppm** (oral - rat –18 mos) **23,500 ppm** (oral - mouse –24 mos)	No data found	No data found
Developmental Toxicity NOAEL =	No data found	No data found	No data found

Table 5. Summary of data for the Benzotriazoles category

Endpoint	1-H-Benzotriazole 95-14-7	1-H-Benzotriazole, 4 (or 5)-methyl 29385-43-1	1-H-Benzotriazole, 4 (or 5)-methyl, sodium salt 64665-57-2
Environmental Fate			
Photodegradation	C	C	C
Hydrolysis	A	R	A/R
Biodegradability	A	A	A
Fugacity	C	C	C
Ecotoxicity			
Acute Fish Toxicity	A	A	A
Acute Invertebrate Toxicity	A	A	A
Algal Toxicity	A	A	A
Mammalian Toxicity			
Acute Toxicity	A	A	A
Repeated Dose	A	A	R
Mutagenicity – gene mutation	A	A	R
Mutagenicity – chromosome aberration	A	A	R
Reproductive Toxicity	A	R	R
Developmental Toxicity	T	R	R

Key for symbols in table:
A = Adequate data available
R = Endpoint requirement fulfilled using category approach, SAR
C = Endpoint requirement fulfilled based on calculated data
T = Testing to be done

References:

Boyer, JH. 1961. "Monocyclic triazoles and Benzotriazoles" in Heterocyclic Compounds. Vol. 7. R.C. Elderfield, Ed. J. Wiley & Sons, Inc., New York.

Meylan, W. and Howard, P. (1999) Syracuse Research Corporation. Environmental Science Center, 6225 Running Ridge Road, North Syracuse, NY 13212-2510.

NTIS PB-266 366. 1977. Investigation of Selected Potential Environmental Contaminants: Benzotriazoles. Syracuse Research Corporation for Environmental Protection Agency, Washington, D.C. Office of Toxic Substances.

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D a t a S e t

Existing Chemical	ID: 64665-57-2
CAS No.	64665-57-2
EINECS Name	sodium 4(or 5)-methyl-1H-benzotriazolide
EINECS No.	265-004-9
Molecular Weight	155
Molecular Formula	C7H6N3.Na

Producer Related Part
Company:
Creation date: 15-JUL-1999

Substance Related Part
Company:
Creation date: 15-JUL-1999

Memo: SOCMA, Benzotriazoles Coalition

Printing date: 06-DEC-2001
Revision date:
Date of last Update: 06-DEC-2001

Number of Pages: 22

Chapter (profile): Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile): Reliability: without reliability, 1, 2, 3, 4
Flags (profile): Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 OECD and Company Information

Type: lead organisation
Name: Synthetic Organic Chemicals Manufacturers Association (SOCMA), Benzotriazoles Coalition
Street: 1850 M Street NW, Suite 700
Town: 20036 Washington, D.C.
Phone: 202-721-4100
Telefax: (202) 296-8120

05-DEC-2001

Type: cooperating company
Name: Bayer Corporation
Country: United States

05-DEC-2001

Type: cooperating company
Name: PMC Specialties Group, Inc.
Country: United States

05-DEC-2001

1.0.2 Location of Production Site
-

1.0.3 Identity of Recipients
-

1.1 General Substance Information

Substance type: organic
Physical status: liquid
05-DEC-2001

1.1.0 Details on Template
-

1.1.1 Spectra
-

1.2 Synonyms

CO-TT85
05-DEC-2001

Cobratec TT-50S
06-DEC-2001

Cobratec TT-85
05-DEC-2001

Preventol CI 7-50
05-DEC-2001

tolyltriazole, sodium salt
05-DEC-2001

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
-

1.9 Source of Exposure
-

1.10.1 Recommendations/Precautionary Measures
-

1.10.2 Emergency Measures
-

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: -5 - -10 degree C
Testsubstance: other TS: 50% aqeous solution of sodium tolyltriazole
05-DEC-2001 (1)

2.2 Boiling Point

Value: ca. 106 degree C at 1013 hPa
Decomposition: yes
Testsubstance: other TS: 50% aqeous solution of sodium tolyltriazole
05-DEC-2001 (1)

2.3 Density

Type: density
Value: 1.18 g/cm3 at 20 degree C
Testsubstance: other TS: 50% aqeous solution of sodium tolyltriazole
05-DEC-2001 (1)

2.3.1 Granulometry

-

2.4 Vapour Pressure

Value: .0000000000067 hPa at 25 degree C
Method: other (calculated): MPBPWIN (v1.31)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Result: Vapor Pressure Estimations (25 deg C):
(Using BP: 555.38 deg C (estimated))
(Using MP: 238.47 deg C (estimated))
VP: 8.02E-015 mm Hg (Antoine Method)
VP: 5.23E-012 mm Hg (Modified Grain Method)
VP: 1.74E-011 mm Hg (Mackay Method)
Selected VP: 5.23E-012 mm Hg (Modified Grain Method)
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
06-DEC-2001 (2)

Value: .0533 hPa at 20 degree C
Testsubstance: other TS: 50% aqeous solution of sodium tolyltriazole
06-DEC-2001 (3)

Value: 25 hPa at 20 degree C
Testsubstance: other TS: 50% aqeous solution of sodium tolyltriazole
06-DEC-2001 (1)

2.5 Partition Coefficient

log Pow: .658
Method: other (calculated): KOWWIN Program (v1.65)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Result: Log Kow(version 1.65 estimate): 0.66

SMILES : [Na]Cc1cccc2c1nnn2
CHEM : 1H-Benzotriazole, 4(or 5)-methyl- sodium salt
MOL FOR: C7 H6 N3 Na1
MOL WT : 155.14

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH2- [aliphatic carbon]	0.4911	0.4911
Frag	6	Aromatic Carbon	0.2940	1.7640
Frag	3	Aromatic Nitrogen [5-member ring]	-0.5262	-1.578
Factor	1	1,2,3-Triazole correction	0.7525	0.7525
Factor	1	{Na,K,Li} [notoxyattach]**questionable!	-1.0000**	-1.0000
Const		Equation Constant		0.2290
NOTE		An estimated coefficient (**) used		

Log Kow = 0.6580

Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
06-DEC-2001 (2)

2.6.1 Water Solubility

Qualitative: miscible
Testsubstance: other TS: 50% aqeous solution of sodium tolyltriazole
06-DEC-2001 (1)

Value: 55 vol% at 20 degree C
06-DEC-2001 (4)

2.6.2 Surface Tension

-

2.7 Flash Point

-

2.8 Auto Flammability

-

2.9 Flammability
-

2.10 Explosive Properties
-

2.11 Oxidizing Properties
-

2.12 Additional Remarks
-

3.1.1 Photodegradation

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1560000 molecule/cm3
Rate constant: .0000000000034188 cm3/(molecule * sec)
Degradation: 50 % after 3.1 day
Method: other (calculated): AOP Program (v1.89)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
06-DEC-2001 (2)

3.1.2 Stability in Water
Remark: Stable. Sodium Tolyltriazole dissolves in water, it does not hydrolyze. Sold as aqueous solution
Flag: Critical study for SIDS endpoint
06-DEC-2001

3.1.3 Stability in Soil
-

3.2 Monitoring Data (Environment)
-

3.3.1 Transport between Environmental Compartments

Type: fugacity model level III
Media: other: air, water, soil, sediment
Air (Level I):
Water (Level I):
Soil (Level I):
Biota (L.II/III):
Soil (L.II/III):
Method: other: EPIWin Level III Fugacity Model
Year: 1999
Result:

Media	Distribution (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	2.32e-006	75.1	1000	3.49e-020
Water	43.5	360	1000	9.65e-022
Soil	56.4	360	1000	4.03e-020
Sediment	0.0754	1.44e+003	0	8e-022

Media	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	0.000272	0.000295	9.08e-006	9.84e-006
Water	1.07e+003	554	35.5	18.5
Soil	1.38e+003	0	46	0
Sediment	0.461	0.0192	0.0154	0.000639

Persistence Time: 424 hr

Reaction Time: 520 hr
Advection Time: 2.3e+003 hr
Percent Reacted: 81.5
Percent Advected: 18.5
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
06-DEC-2001 (2)

3.3.2 Distribution
-

3.4 Mode of Degradation in Actual Use
-

3.5 Biodegradation

Type: aerobic
Inoculum:
Degradation: ca. 70 % after 28 day
Method: Directive 87/302/EEC, part C, p. 99 "Biodegradation: Zahn-Wellens test"
Year: GLP: no data
Test substance: other TS: 50% aqeous solution of sodium tolyltriazole
06-DEC-2001 (1)

Type: aerobic
Inoculum:
Method:
Year: GLP:
Test substance:
Remark: See IUCLILD data set on methyl-1H-benzotriazole (CAS# 29385-43-1).
06-DEC-2001

3.6 BOD5, COD or BOD5/COD Ratio
-

3.7 Bioaccumulation
-

3.8 Additional Remarks
-

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: static
Species: Lepomis macrochirus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: Analytical monitoring:
NOEC: 34
LC50: > 173
Method:
Year: GLP: yes
Test substance: other TS: 50% sodium tolyltriazole in water
Method: Bluegill sunfish (initial bw = 5.0g) were acclimated for at least 5 days. During the experiment, the fish were not fed. On Day 0, 10 fish were introduced into test chambers containing nominal concentrations of 15, 23, 34, 51, 77, 115, and 173 ppm test substance. Fish were observed daily for mortality and signs of intoxication.
Remark: Concentration in ppm
Result: LC50 (96 hr) = > 173 ppm
NOEC = 34 ppm

Conc	#fish	Mortality/ signs of intoxication 24	48	72	96 (hours)
Control	20	0/0	0/0	0/0	0/0
15 ppm	10	0/0	0/0	0/0	0/0
23 ppm	10	0/0	0/0	0/0	0/0
34 ppm	10	0/0	0/0	0/0	0/0
51 ppm	10	0/7	0/4	0/3	0/0
77 ppm	10	1/9	1/9	1/9	1/9
115 ppm	10	0/10	0/10	0/10	0/10
173 ppm	10	0/10	0/10	0/10	0/10

Clinical signs were present at Concentrations from 53 to 173. In general, the fish were either at the surface or on the bottom and exhibited almost total inactivity, but were hyperreactive to stimuli. Fish in the 51ppm group recovered by 96 hours, but none did in the higher concerntrations. One fish died in the 77ppm group, which appears to be an unusual sensitivity since there were no deaths at the two higher concentrations.
Test condition: Water temperature and dissolved Oxygen measured daily; pH measured at beginning and end of study; hardness and alkalinity measured at beginning of study.

Photoperiod = 16 hours light/day
Temperature: 15 - 18 degree C
pH: 7.1 - 7.8
Dissolved Oxygen: 5.4 - 8.4 mg/l
Hardness: 143 - 147 mg/l
Alkalinity: 54 - 55 mg/l
Aeration: none
Reliability: (1) valid without restriction
GLP study, Meets generally accepted scientific method and is

described in sufficient detail
Flag: Critical study for SIDS endpoint
06-DEC-2001 (5)

Type:
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC50: ca. 25
Method:
Year: GLP: yes
Test substance: other TS: 50% sodium tolyltriazole in water
Method: Rainbow trout (initial bw of 1.21 - 1.35g) were acclimated for at least 5 days. During the experiment, the fish were not fed and the water was not aerated. On Day 0, 10 fish were introduced into test chambers containing nominal concentrations of 16.6, 19.9, 23.2, 27.4, 32.5, 38.4, and 53.8 ppm test substance. Fish were observed daily for mortality and signs of intoxication.
LC50 and 95% confidence limits were calculated according to Weil CS. 1952. Biometrics. 8:249.
Remark: Concentration in ppm
Result: LC50 (24 hr) = > 53.8 ppm
LC50 (48 hr) = 33 (31-35) ppm
LC50 (72 hr) = 31 (29-32) ppm
LC50 (96 hr) = 25 (24-26) ppm

Conc	#fish	Mortality/ signs of intoxication 24	48	72	96 (hours)
Control	20	0/0	0/0	0/0	0/0
16.6 ppm	10	0/0	0/0	0/0	0/0
19.9 ppm	10	0/0	0/1	0/4	0/4*
23.2 ppm	10	0/0	0/10	1/9*	1/9*
27.4 ppm	10	0/2	0/10*	0/10*	10/-*
32.5 ppm	10	0/10	9/1*	9/1*	9/1*
38.4 ppm	10	0/9	5/5*	9/1*	10/-
53.8 ppm	10	0/10	10/-*	10/-	10/-

* mortality values used to calculate the LC50.
Test condition: Water temperature and dissolved Oxygen measured daily; pH measured at beginning and end of study; hardness and alkalinity measured at beginning of study.

Photoperiod = 16 hours light/day
Temperature: 9.0 - 12.3 degree C
pH: 7.1 - 8.6
Dissolved Oxygen: 3.4 - 18.8 mg/l
Hardness: 151 - 163 mg/l
Alkalinity: 56 - 70 mg/l
Reliability: (1) valid without restriction
GLP study, Meets generally accepted scientific method and is described in sufficient detail
Flag: Critical study for SIDS endpoint
06-DEC-2001 (6)

Type:
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC0: 100
LC50: 122
Method:
Year: GLP:
Test substance: other TS: 50% sodium tolyltriazole in water
06-DEC-2001 (1)

Type:
Species: Lepomis macrochirus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 191.2
Method:
Year: GLP:
Test substance: other TS: 50% Sodium Tolyltriazole in water
06-DEC-2001 (4)

Type:
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 23.7
Method:
Year: GLP:
Test substance: other TS: 50% Sodium Tolyltriazole in water
06-DEC-2001 (4)

Type: other: calculated
Species: other
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 137 - 179
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Remark: Chemical may not be soluble enough to measure this predicted effect.
Result: ECOSAR v0.99e Class(es) Found

Benzotriazoles

Predicted ECOSAR Class	Organism	Duration	End Pt	mg/L
Neutral Organic SAR: Fish (Baseline Toxicity)		14-day	LC50	3060.916
Benzotriazoles: Fish [CLOGP]		96-hr	LC50	179.610
Benzotriazoles: Fish [SRC]		96-hr	LC50	137.079
Benzotriazoles: Fish [CLOGP]			ChV	51.989

Benzotriazoles: Fish [SRC] ChV 12.658
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
06-DEC-2001 (2)

4.2 Acute Toxicity to Aquatic Invertebrates

Type: static
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring:
NOEC: 100
LC50 : 280
Method: other: according to TSCA Public Law 94-469 (1976) and USEPA Registration of Pesticides guidelines Fed. Reg. 07/10/78:29696-29741(1978)
Year: 1978 GLP: yes
Test substance: other TS: 50% aqeous solution of sodium tolyltriazole
Result: LC50 (24 hr) = 440 mg/l (320-560)
LC50 (48 hr) = 280 mg/l (180-560)
NOEC = 100 mgl

Conc	Mortality/ total # Daphnia 24	48 (hours)
Control	0/20	0/20
100 mg/l	0/20	0/20
180 mg/l	0/20	0/20
320 mg/l	0/20	14/20
560 mg/l	19/20	20/20
1000 mg/l	20/20	20/20

Clinical signs present at 180 mg/l were erratic behavior; at 320 mg/l Daphnia were either at the surface or on the bottom; and at 560 mg/l one exhibited loss of equilibrium.
Test condition: Water temperature, pH, and dissolved Oxygen measured at beginning and end of study; hardness and alkalinity measured at beginning of study.

Photoperiod = 16 hours light/day
Temperature: 20 degree C
pH: 8.3 - 8.8
Dissolved Oxygen: 7.4 - 8.1 mg/l
Hardness: 225 - 275 ppm
Alkalinity: 325 - 375 ppm
Reliability: (1) valid without restriction
GLP, National standards method
Flag: Critical study for SIDS endpoint
06-DEC-2001 (7)

Type:
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring:
LC50 : 245.7
Method:
Year: GLP:
Test substance:
06-DEC-2001 (4)

Type: other: calculated
Species: Daphnia sp. (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 596 - 1225
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Remark: Chemical may not be soluble enough to measure this predicted effect.
Result: ECOSAR v0.99e Class(es) Found

Benzotriazoles

Predicted ECOSAR Class	Organism	Duration	End Pt	mg/L
Benzotriazoles:	Daphnid [CLOGP]	48-hr	LC50	1225.382
Benzotriazoles:	Daphnid [SRC]	48-hr	LC50	596.721
Benzotriazoles:	Daphnid [CLOGP]		ChV	30.333
Benzotriazoles:	Daphnid [SRC]		ChV	8.853

Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
06-DEC-2001 (2)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Selenastrum capricornutum (Algae)
Endpoint: growth rate
Exposure period: 96 hour(s)
Unit: Analytical monitoring:
NOEC: 10
EC50: 26.2
Method:
Year: GLP: yes
Test substance: other TS: 50% aqeous solution of sodium tolyltriazole
Method: Selenastrum capricornutum (2x10 e4 cells/ml) were exposed to test solutions of 0, 10, 30, 90, 270, and 810 mg/l (nominal concentrations) for four days and observed during a four day withdrawal period. Growth was monitored by cell counts and estimated biomass.

Comparison of cell numbers and biomass during exposure and withdrawal were made using Duncan's multiple range test with alpha = 0.05. Dose-response analysis was done by probit method using log nominal concentrations. Biomass was estimated as: biomass (mg)= # cells x cell volume x 3.6 x 10 e-7.
Remark: Concentration in ppm
Result: Growth EC50 (96hr) = 26.2 ppm (16.6- 36.7)
Biomass EC50 (96hr) = 32.0 ppm (4.1 - 78.7)
NOEC = 100 ppm
Lowest algastatic concentration = 270 ppm
No level tested was algacidal.

Conc	cell counts 0	4	8 (days)
Control			
A	488	2211	26626
B	474	9017	60244
C	449	13473	58829
10 ppm			
A	584	4868	
B	551	8907	
C	602	3450	
30 ppm			
A	414	4809	63350
B	501	3850	54189
C	530	2620	51315
90 ppm			
A	454	2017	54920
B	551	1548	54570
C	501	3066	59239
270 ppm			
A	592	619	19552
B	483	180	23932
C	369	129	12171
810 ppm			
A	575	436	4071
B	609	291	2022

C 488 165 2008

Test condition: The cultures were kept at 26-27 degree C with 400 +/-40 footcandles continuous cool-white fluorescent illumination and were continually oscillated on a platform at 100 rpm. Each concentration was tested in triplicate.

Reliability: (1) valid without restriction
GLP study, Meets generally accepted scientific method and is described in sufficient detail

Flag: Critical study for SIDS endpoint

06-DEC-2001 (8)

Species: other algae
Endpoint:
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 50 - 56
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure

Result:

ECOSAR Class	Organism	Duration	End Pt	mg/L
Benzotriazoles:	Green Algae [CLOGP]	96-hr	EC50	56.779
Benzotriazoles:	Green Algae [SRC]	96-hr	EC50	50.768
Benzotriazoles:	Algae [CLOGP]		ChV	12.608
Benzotriazoles:	Algae [SRC]		ChV	7.153

Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint

06-DEC-2001 (2)

4.4 Toxicity to Microorganisms e.g. Bacteria
-

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish
-

4.5.2 Chronic Toxicity to Aquatic Invertebrates
-

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms
-

4.6.2 Toxicity to Terrestrial Plants
-

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 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Strain: Wistar
Sex: male/female
Number of Animals: 10
Vehicle:
Value: ca. 1980 mg/kg bw
Method:
Year: 1983 GLP: no data
Test substance: other TS: 50% sodium tolyltriazole in water
Method: 5 rats/sex/dose, 5 doses: 1.0, 1.3, 1.6, 1.8, 2.5, 2.8 ml/kg bw, given by gavage, observation time: 14 d, pathologic examination of rats that died during observation time and of the survivors after termination.
Remark: signs of intoxication: reduced general condition, prone position, rough fur, sedation.
Pathologic examination:
decedents: corrosion of the gastric mucous membranes;
survivors: no findings.
LD50: 1.66 ml/kg bw (ca. 1980 mg/kg bw)
Reliability: (2) valid with restrictions
Meets generally accepted scientific method and is described in sufficient detail.
Flag: Critical study for SIDS endpoint
06-DEC-2001 (9)

Type: LD50
Species: rat
Strain:
Sex: male
Number of Animals:
Vehicle:
Value: ca. 920 mg/kg bw
Method:
Year: GLP:
Test substance: other TS: 50% sodium tolyltriazole in water
06-DEC-2001 (4) (1)

Type: LD50
Species: rat
Strain:
Sex: female
Number of
Animals:
Vehicle:
Value: 640 - 735 mg/kg bw
Method:
Year: GLP:
Test substance: other TS: 50% sodium tolyltriazole in water
06-DEC-2001 (4) (1)

5.1.2 Acute Inhalation Toxicity
-

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rabbit
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: > 2000 mg/kg bw
Method:
Year: GLP:
Test substance: other TS: 50% sodium tolyltriazole in water
Remark: 24 hours of exposure; rabbits exhibited no symptoms
03-OCT-2000 (1)

5.1.4 Acute Toxicity, other Routes
-

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Concentration: undiluted

Exposure: Semiocclusive
Exposure Time: 4 hour(s)
Number of Animals: 3
PDII:
Result: corrosive
EC classificat.:
Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year: 1983 GLP: no data
Test substance: other TS: 50% aqeous solution of sodium tolyltriazole
Reliability: (1) valid without restriction
Guideline study
06-DEC-2001 (10)

5.2.2 Eye Irritation
-

5.3 Sensitization
-

5.4 Repeated Dose Toxicity
Remark: Repeat dose studies (28 d or 18-24 month studies) conducted with tolyl triazole (29385-43-1) and 1H-Benzotriazole(95-14-7)

demonstrated an apparent reduction in toxicity with increasing molecular weight. The repeat dose toxicity of the sodium salt (CAS#64665-57-2) is expected to be similar to the repeat dose toxicity of tolyl triazole (29385-43-1) NOAEL = 150 mg/kg bw (oral- rat - 29 D) since the Sodium salt will dissociate to the methyl benzotriazole in aqueous solution.
06-DEC-2001 (11)

5.5 Genetic Toxicity 'in Vitro'
Remark: Mutagenicity testing has been conducted on tolyl triazole (29385-43-1) and 1H-Benzotriazole(95-14-7). The weight of evidence for the members of this category indicates these chemicals are not mutagenic or clastogenic. By bridging existing data to the sodium salt, which will dissociate to the

methyl benzotriazole in aqueous solution, the mutagenicity aspect of the category has been evaluated adequately.
06-DEC-2001 (11)

5.6 Genetic Toxicity 'in Vivo'

Remark: Mouse micronucleus tests have been conducted on tolyl triazole (29385-43-1) and 1H-Benzotriazole(95-14-7). Both resulted in Negative results. There are also carcinogenicity studies on 1H-Benzotriazole(95-14-7). By bridging existing data to the sodium salt, which will dissociate to the methyl benzotriazole in aqueous solution, the mutagenicity aspect of the category has been evaluated adequately.

06-DEC-2001 (11)

5.7 Carcinogenicity

-

5.8 Toxicity to Reproduction

Remark: The 78 week oral study of 1H-benzotriazole (95-14-7) in Fischer 344 rats and the 104 week oral study of 1H-benzotriazole in B6C3F1 mice did not find any evidence of pathology in the reproductive organs. The organs examined were: prostate/testis/epididymis of males and uterus/ovaries of females.

06-DEC-2001 (12)

5.9 Developmental Toxicity/Teratogenicity

-

5.10 Other Relevant Information

-

5.11 Experience with Human Exposure

-

(1) Safety Data Sheet Bayer AG, 09.02.1999

(2) Meylan W. and Howard P. (1999) EPIWin Modeling Program. Syracuse Research Corporation. Environmental Science Center, 6225 Running Ridge Road, North Syracuse, NY 13212-2510.

(3) PMC Specialties Group, Inc., MSDS 08/16/99

(4) PMC Specialties Group, Inc., MSDS 01/29/97

(5) Study No. 84-066-02. Mobay Chemical Corporation. August 3, 1984.

(6) Study No. 84-066-01. Mobay Chemical Corporation. June 15, 1984.

(7) Analytical Bio-Chemistry Laboratories, Inc. Report #32028. August 24,1984.

(8) Study No. 84-060-02. Mobay Chemical Corporation. August 2, 1984.

(9) Bayer AG data, E. Löser: Untersuchungen zur akuten oralen Toxizität an männlichen und weiblichen Ratten, June 1983.

(10) Bayer AG data, Suberg H., Prüfung auf primär reizende/ätzende Wirkung an der Kaninchenhaut, January, 1984

(11) IUCLID data sets on CAS Nos. 95-14-7 and 29385-43-1

(12) NTIS PB#285202 March, 1978. Bioassay of 1H-benzotriazole for possible carginogenicity. CAS No. 95-14-7

7.1 End Point Summary

-

7.2 Hazard Summary

-

7.3 Risk Assessment

-

I U C L I D

D a t a S e t

Existing Chemical	ID: 95-14-7
CAS No.	95-14-7
EINECS Name	benzotriazole
EINECS No.	202-394-1
Molecular Weight	119.1
Molecular Formula	C6H5N3

Producer Related Part
  Company:
  Creation date: 15-JUL-1999

Substance Related Part
  Company:
  Creation date: 15-JUL-1999

Memo: SOCMA, Benzotriazoles Coalition

Printing date: 26-DEC-2001
Revision date:
Date of last Update: 26-DEC-2001

Number of Pages: 35

Chapter (profile): Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile): Reliability: without reliability, 1, 2, 3, 4
Flags (profile): Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 OECD and Company Information

Type: lead organisation
Name: Synthetic Organic Chemical Manufacturers Association, Benzotriazoles Coalition
Street: 1850 M Street N.W., Suite 700
Town: 20036 Washington, D.C.
Country: United States
Phone: (202) 721-4100
Telefax: (202) 296-8120

03-DEC-2001

Type: cooperating company
Name: Bayer Corporation
Country: United States

03-DEC-2001

Type: cooperating company
Name: PMC Specialties Group, Inc.
Country: United States

03-DEC-2001

1.0.2 Location of Production Site
-

1.0.3 Identity of Recipients
-

1.1 General Substance Information

Substance type: organic
Physical status: solid
Purity: ca. 100 % w/w
04-DEC-2001

1.1.0 Details on Template
-

1.1.1 Spectra
-

1.2 Synonyms

1,2,3-BENZOTRIAZOLE
03-DEC-2001

BENZOTRIAZOLE
03-DEC-2001

Cobratec 99
Source: PMC Specialties Group
03-DEC-2001

Preventol CI 8-100
Source: Bayer Corporation
03-DEC-2001

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
-

1.9 Source of Exposure
-

1.10.1 Recommendations/Precautionary Measures
-

1.10.2 Emergency Measures
-

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: 100 degree C
Method: other: Handbook value
GLP: no data
Testsubstance: other TS: 1H-benzotriazole; purity not noted
Reliability: (2) valid with restrictions
Data from Handbook or collection of data
Flag: Critical study for SIDS endpoint
04-DEC-2001 (1)

Value: 94 - 99 degree C
Testsubstance: other TS: 1H-benzotriazole; purity >99%
Remark: stock point
04-DEC-2001 (2) (3)

2.2 Boiling Point

Value: 204 degree C at 20 hPa
Method: other: Handbook value
GLP: no data
Testsubstance: other TS: 1H-benzotriazole; purity not noted
Reliability: (2) valid with restrictions
Data from Handbook or collection of data
Flag: Critical study for SIDS endpoint
04-DEC-2001 (1)

Value: > 200 degree C
Testsubstance: as prescribed by 1.1 - 1.4
04-DEC-2001 (3)

Value: > 300 degree C
Testsubstance: other TS: 1H-benzotriazole; purity >99%
04-DEC-2001 (2)

2.3 Density

Type: density
Value: ca. 1.19 g/cm3 at 100 degree C
Testsubstance: as prescribed by 1.1 - 1.4
Remark: mellifluousness
Flag: Critical study for SIDS endpoint
04-DEC-2001 (3)

Type: bulk density
Value: ca. 500 kg/m3
Testsubstance: as prescribed by 1.1 - 1.4
04-DEC-2001 (3)

2.3.1 Granulometry

-

2.4 Vapour Pressure

Value: .000797 hPa at 25 degree C
Method: other (calculated): MPBPWIN (v1.31)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
04-DEC-2001 (4)

Value: ca. .00001 hPa at 25 degree C
Testsubstance: as prescribed by 1.1 - 1.4
04-DEC-2001 (3)

Value: .0533 hPa at 20 degree C
Testsubstance: other TS: 1H-benzotriazole; purity >99%
Flag: Critical study for SIDS endpoint
04-DEC-2001 (2)

2.5 Partition Coefficient

log Pow: 1.34 at 22.7 degree C
Method: other (measured)
Year: 1991
GLP: yes
Testsubstance: as prescribed by 1.1 - 1.4
Reliability: (1) valid without restriction
GLP study
Flag: Critical study for SIDS endpoint
04-DEC-2001 (5)

log Pow: 1.167 at 25 degree C
Method: other (calculated): KOWWIN Program (v1.65)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Result: Experimental Database Structure Match:
Name : 1H-Benzotriazole
CAS Num : 000095-14-7
Exp Log P: 1.44
Exp Ref : Hansch et al; 1995

Experimental Database Structure Match:
Name : 2H-Benzotriazole
CAS Num : 000273-02-9
Exp Log P: 1.44
Exp Ref : Sangster 1993

SMILES : c1ccc2nnnc2c1
CHEM : 1H-Benzotriazole
MOL FOR: C6 H5 N3
MOL WT : 119.13

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	6	Aromatic Carbon	0.2940	1.7640
Frag	3	Arom. Nitrogen [5-member ring]	-0.5262	-1.5786
Factor	1	1,2,3-Triazole correction	0.7525	0.7525
Const		Equation Constant		0.2290

Log Kow = 1.1669

Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
04-DEC-2001 (4)

log Pow: 1.44
Method: other (measured)
Year:
GLP: no data
Testsubstance: other TS: 1H-Benzotriazole (CAS 95-14-7;) purity not noted
09-MAY-2001 (6)

2.6.1 Water Solubility

Value: 1 - 5 mg/l at 23.7 degree C
Method: other: no data
GLP: no data
Testsubstance: other TS: 1-H-benzotraizole; purity not noted
Reliability: (2) valid with restrictions
Data from Handbook or collection of data
Flag: Critical study for SIDS endpoint
04-DEC-2001 (7)

Value: ca. 19 g/l at 20 degree C
Qualitative: miscible
Testsubstance: other TS: 1H-benzotriazole; purity not noted
Reliability: (2) valid with restrictions
Data from Handbook or collection of data
04-DEC-2001 (8) (3)

Qualitative: slightly soluble (0.1-100 mg/L)
Method: other: Handbook value
GLP: no data
Testsubstance: other TS: 1H-benzotriazole; purity not noted
Reliability: (2) valid with restrictions
Data from Handbook or collection of data
Flag: Critical study for SIDS endpoint
04-DEC-2001 (1)

Value: 2 vol% at 20 degree C
Testsubstance: other TS: 1H-benzotriazole; purity >99%
04-DEC-2001 (2)

pKa: 8.2 at 25 degree C
Remark: The reaction suggests that benzotriazole will be less soluble in pH <7 (such as rainwater) and more soluble in solutions >7 (such as seawater) than in distilled water. Benzotriazole reacts with solutions of alkali metal hydroxides producing soluble alkali salts.
26-DEC-2001 (9)

2.6.2 Surface Tension
-

2.7 Flash Point

Value: ca. 195 degree C
Type:
Method: other: DIN 51584
Year:
Testsubstance: as prescribed by 1.1 - 1.4
04-DEC-2001 (3)

2.8 Auto Flammability
-

2.9 Flammability

Result:
Method: other: DIN 51794
Testsubstance: as prescribed by 1.1 - 1.4
Remark: ignition temperature: ca. 400 degrees C
04-DEC-2001 (3)

2.10 Explosive Properties
-

2.11 Oxidizing Properties
-

2.12 Additional Remarks
-

3.1.1 Photodegradation

```
Type:             air
INDIRECT PHOTOLYSIS
  Sensitizer:     OH
  Conc. of sens.: 1560000 molecule/cm3
  Rate constant:  .000000000001 cm3/(molecule * sec)
  Degradation:    50 % after 10.7 day
Method:           other (calculated): AOP Program (v1.89)
  Year:           1999                          GLP: no
Test substance:   other TS: molecular structure
Result:           AOP Program (v1.89) Results:
                  ============================
                  SMILES : c1ccc2nnnc2c1
                  CHEM   : 1H-Benzotriazole
                  MOL FOR: C6 H5 N3
                  MOL WT : 119.13
                  --------- SUMMARY (AOP v1.89): HYDROXYL RADICALS ----------
                  Hydrogen Abstraction       =   0.0000 E-12 cm3/molecule-sec
                  Reaction with N, S and -OH =   0.0000 E-12 cm3/molecule-sec
                  Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
                  Addition to Olefinic Bonds =   0.0000 E-12 cm3/molecule-sec
                  Addition to Aromatic Rings =   0.0000 E-12 cm3/molecule-sec
                  **Addition to Fused Rings  =   1.0000 E-12 cm3/molecule-sec

                     OVERALL OH Rate Constant =   1.0000 E-12 cm3/molecule-sec
                     HALF-LIFE =    10.696 Days (12-hr day; 1.5E6 OH/cm3)
Reliability:      (2)  valid with restrictions
                  Accepted calculation method
Flag:             Critical study for SIDS endpoint
04-DEC-2001                                                                (4)
```

3.1.2 Stability in Water
-

3.1.3 Stability in Soil
-

3.2 Monitoring Data (Environment)
-

3.3.1 Transport between Environmental Compartments

Type: fugacity model level III
Media: other: air - water - sediment- soil
Air (Level I):
Water (Level I):
Soil (Level I):
Biota (L.II/III):
Soil (L.II/III):
Method: other: EPIWIN Level III Fugacity Model
Year: 1999
Result:

Media	Distribution (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	4.6	257	1000	9.95e-011
Water	42.3	360	1000	5.94e-012
Soil	53.1	360	1000	1.45e-010
Sediment	0.0869	1.44e+003	0	4.8e-012

Media	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	131	485	4.37	16.2
Water	859	446	28.6	14.9
Soil	1.08e+003	0	35.9	0
Sediment	0.442	0.0184	0.0147	0.000612

Persistence Time: 352 hr
Reaction Time: 510 hr
Advection Time: 1.13e+003 hr
Percent Reacted: 68.9
Percent Advected: 31.1

Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
04-DEC-2001 (4)

3.3.2 Distribution
-

3.4 Mode of Degradation in Actual Use
-

3.5 Biodegradation

Type: aerobic
Inoculum: activated sludge, industrial, non-adapted
Concentration: 2 mg/l related to Test substance
Degradation: 90 % after 28 day
Testsubstance:

3 hour(s)	27 %
7 day	55 %
14 day	75 %
21 day	83 %
27 day	85 %

Method: other: DIN 38 412 L 25 (Zahn-Wellens Test)
Year: 1988 GLP: no
Test substance: as prescribed by 1.1 - 1.4
Remark: analytical monitoring of primary degradation
Result: primary degradation with daylight: 90 % after 28 days
degradation without daylight: 83 % after 28 days
Reliability: (1) valid without restriction
Meets National standards method (AFNOR/DIN)
Flag: Critical study for SIDS endpoint
04-DEC-2001 (10)

Type: aerobic
Inoculum: predominantly domestic sewage, adapted
Degradation: 0 % after 28 day
Method: OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
Year: 1985 GLP: no
Test substance: as prescribed by 1.1 - 1.4
Remark: Test concentrations: 2.4, 8, 24, 80 mg/l
Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint
04-DEC-2001 (11)

Type: aerobic
Inoculum:
Degradation: 0 % after 20 day
Controlsubstance: Aniline
Kinetic: 17 day 100 %
Method: other: River Die-Away Test
Year: GLP: no data
Test substance: other TS: Cobratec 99; purity >99%
04-DEC-2001 (12)

3.6 BOD5, COD or BOD5/COD Ratio

Remark: ThoD: 1948 mg/g
COD: 1376 mg/g
04-DEC-2001 (13)

3.7 Bioaccumulation
-

3.8 Additional Remarks

Remark: Elective cultures and continuous enrichment failed to demonstrate biodegradation of benzotriazole.
Organisms were elected from soil samples from around Cardiff, activated sludge from a coke oven liquor treatment plant, microbially contaminated liquor wastes from a manufacturer of benzotriazole derivatives, microbially contaminated ship's engine cooling waters.
No organisms that could be demonstrated to utilize benzotriazole for growth in solid or liquid minimal media were isolated from a small recirculating plant (TS conc. increased in the main tank (6 l, vigorously stirred and aerated, at ambient temp. 8 - 24 degrees C) from 0.5 to 3 mM in steps over 80 days of continuous operation and a proprietary anti-corrosion additive that contains benzotriazole).
The minimum inhibitory conc. of the TS was estimated at 20 mM.
Source: Bayer AG Leverkusen
04-DEC-2001 (14)

AQUATIC ORGANISMS

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: 100
LC50: > 100
Method: other: "Letale Wirkung beim Zebrabaerbling - Brachydanio rerio" (LC 0, LC 50, LC 100; 48-96 Stunden), Verfahrensvorschlag Umweltbundesamt, Mai 1984
Year: 1984 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Result:

time (hr)	Abnormal swimming habit	Mortality
24	3/10	0/10
48	10/10	0/10
72	10/10	0/10
96	10/10	0/10

Test condition:

time (hr)	temp (degree C)	O2 (mg/l)	pH
0	19.6	9.8	6.5
24	23.0	9.3	6.7
48	22.0	9.7	6.8
72	22.5	9.3	6.9
96	22.6	8.0	7.0

Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
04-DEC-2001 (15)

Type:
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no data
LC50: 39
EC50 : 24.4
Method: other: Batelle Protocol
Year: GLP: no data
Test substance: other TS: Cobratec 99; purity >99%
Remark: LC50 generated by Binomial method; 95% confidence limits = 28.4- 49.5 mg/l
EC50 generated by Binomial method; 95% confidence limits = 21.0- 28.4 mg/l
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
04-DEC-2001 (12)

Type: flow through
Species: Lebistes reticulatus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 28
Method:
Year: GLP: no data
Test substance: other TS: 1H-benzotriazole; purity not noted
Reliability: (2) valid with restrictions
04-DEC-2001 (16)

Type: flow through
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 28
Method:
Year: GLP: no data
Test substance: other TS: 1H-benzotriazole; purity not noted
Reliability: (2) valid with restrictions
04-DEC-2001 (16)

Type: flow through
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 12
Method:
Year: GLP: no data
Test substance: other TS: 1H-benzotriazole; purity not noted
Remark: fingerlings
04-DEC-2001 (16)

Type: static
Species: Lepomis macrochirus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 25
Method:
Year: GLP: no data
Test substance: other TS: 1H-benzotriazole; purity not noted
Reliability: (2) valid with restrictions
04-DEC-2001 (16)

Type: static
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 25
Method:
Year: GLP: no data
Test substance: other TS: 1H-benzotriazole; purity not noted
Reliability: (2) valid with restrictions
04-DEC-2001 (16)

Type: flow through
Species: Lepomis macrochirus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: Analytical monitoring: no data
TLm : 25
Method:
Year: GLP: no
Test substance: other TS: Benzotriazole (BT-D); purity not noted
Result: Median Tolerance Limit (TLm) = 27.5 ppm (48 hrs); 25.0 ppm (96 hrs)
04-DEC-2001 (17)

Type: flow through
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: Analytical monitoring: no data
TLm : 28
Method:
Year: GLP: no
Test substance: other TS: Benzotriazole (BT-D); purity not noted
Result: Median Tolerance Limit (TLm) = 30.2 ppm (48 hrs); 28.0 ppm (96 hrs)
04-DEC-2001 (17)

Type: flow through
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: Analytical monitoring: no data
Tlm : 12
Method:
Year: GLP: no
Test substance: other TS: Benzotriazole (BT-D); purity not noted
Result: Median Tolerance Limit (TLm) = 15 ppm (48 hrs); 12 ppm (96 hrs)
04-DEC-2001 (17)

Type: static
Species: Lepomis macrochirus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: Analytical monitoring: no data
TLm : 25
Method: EPA OTS 797.1400
Year: GLP: no
Test substance: other TS: Benzotriazole (BT-D); purity not noted
Result: Median Tolerance Limit (TLm) = 27.5 ppm (48 hrs); 25.0 ppm (96 hrs)
04-DEC-2001 (17)

Type: static
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: Analytical monitoring: no data
TLm : 28
Method:
Year: GLP: no
Test substance: other TS: Benzotriazole (BT-D); purity not noted
Result: Median Tolerance Limit (TLm) = 30.2 ppm (48 hrs); 28.0 ppm (96 hrs)
04-DEC-2001 (17)

4.2 Acute Toxicity to Aquatic Invertebrates

Type: static
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
EC0: 63
EC50: 91
EC100: 250
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: 1991 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Result:

Nominal Conc (mg/l)	% immobilization 24 hr	48 hr
0	0	0
63	0	0
88	25	60
125	40	90
177	40	95
250	50	100
354	100	
500	100	

Reliability: (1) valid without restriction
GLP Guideline study
Flag: Critical study for SIDS endpoint
04-DEC-2001 (18)

Type:
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no data
LC50 : 141.6
Method: other: Battelle protocols
Year: GLP: no data
Test substance: other TS: Cobratec 99; purity >99%
Remark: LC50 generated by Probit method; 95% confidence limits = 127.7- 173.5 mg/l
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
04-DEC-2001 (12)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Scenedesmus subspicatus (Algae)
Endpoint: growth rate
Exposure period: 72 hour(s)
Unit: mg/l Analytical monitoring: no
EC10: 58
EC50: 231
Method: other: DIN 38412 L 9
Year: 1992 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Result:

Nominal Conc (mg/l)	% inhibition (72 hr)
0	0
1	0
3.2	0
10	0
32	0
100	8.3
320	91.7
1000	100.0

Reliability: (1) valid without restriction
GLP Guideline study
Flag: Critical study for SIDS endpoint
04-DEC-2001 (19)

Species: Scenedesmus subspicatus (Algae)
Endpoint: biomass
Exposure period: 72 hour(s)
Unit: mg/l Analytical monitoring: no
EC10: 20
EC50: 102
Method: other: DIN 38412 L 9
Year: 1992 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Result:

Nominal Conc (mg/l)	% inhibition (72 hr)
0	0
1	2.7
3.2	2.0
10	0.7
32	10.7
100	47.6
320	96.3
1000	100.0

Reliability: (1) valid without restriction
GLP Guideline study
Flag: Critical study for SIDS endpoint
04-DEC-2001 (19)

Species: other aquatic plant: algae
Endpoint:
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no data
NOEC: 4.1
LOEC: 8
EC50: 15.4
Method: other: Battelle protocol
Year: GLP: no data
Test substance: other TS: Cobratec 99; purity >99%
Remark: EC50 generated by Probit method; 95% confidence limits = 2.5-44.7 mg/l

NOEC and LOEC generated by ANOVA, Bonferroni test
04-DEC-2001 (12)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type: aquatic
Species: activated sludge
Exposure period: 3 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 1060
EC95 : 3800
EC05 : 298
Method: ISO 8192 "Test for inhibition of oxygen consumption by activated sludge"
Year: 1991 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: direct weight
Result:

Nominal Conc (mg/l)	% inhibition
180	0
320	8.3
560	15
1000	50
1800	75

Reliability: (1) valid without restriction
GLP Guideline study
04-DEC-2001 (20)

Type: other
Species: activated sludge of a predominantly domestic sewage
Exposure period: 5 day
Unit: mg/l Analytical monitoring:
EC0: 13.2
Method: other: Standard BOD test: Standard Methods for Examination of Water and Wastewater,13th edition
Year: GLP:
Test substance: other TS: benzotriazole; purity not noted
Result: Concentrations of 0.66 to 13.2 mg/l benzotriazole did not affect the survival of the microbial seed during the 5 day test incubation at 20 degree C.

Sample Conc. (mg/l)		Colony count /ml
0	(initial)	54,570
0	(5 day)	151,000
0.66	(5 day)	207,000
3.3	(5 day)	217,000
6.6	(5 day)	183,000
13.2	(5 day)	164,000

Reliability: (1) valid without restriction
Guideline study
04-DEC-2001 (21)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

-

4.5.2 Chronic Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)
Endpoint: other: immobilisation
Exposure period: 21 day
Unit: mg/l Analytical monitoring: yes
EC50: 76.9
NOEC : 25.9
Method: OECD Guide-line 202, part 2 "Daphnia sp., Reproduction Test"
Year: 1994 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Method: semi-static
analytical monitoring: TOC
To produce the stock solution, the test substance was weighed into water and treated for 1 hour in an ultrasonic device and, subsequently stirred for 1 hour with a magnetic stirrer.
Result: arithmetical mean of analytical values:
EC50: 76.9 mg/l (test substance) corresp. to 47.3 mg/l TOC
Reliability: (1) valid without restriction
GLP Guideline study
04-DEC-2001 (22)

Species: Daphnia magna (Crustacea)
Endpoint: reproduction rate
Exposure period: 21 day
Unit: mg/l Analytical monitoring: yes
NOEC: 25.9
LOEC: 76.9
EC50: 25.9 - 76.9
Method: OECD Guide-line 202, part 2 "Daphnia sp., Reproduction Test"
Year: 1993 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: semi-static
analytical monitoring: TOC
To produce the stock solution the test substance was weighed into water and treated for 1 hour in an ultrasonic device and, subsequently stirred for 1 hour with a magnetic stirrer.
Result: arithmetical mean of analytical values:
EC50: 25.9 mg/l (test substance) corresp. to 15.3 mg/l TOC
76.9 mg/l (test substance) corresp. to 47.3 mg/l TOC
NOEC: 25.9 mg/l (test substance) corresp. to 15.3 mg/l TOC
LOEC: 76.9 mg/l (test substance) corresp. to 47.3 mg/l TOC
Reliability: (1) valid without restriction
GLP Guideline study
04-DEC-2001 (22)

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms
-

4.6.2 Toxicity to Terrestrial Plants
-

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 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Strain: no data
Sex: male/female
Number of Animals: 10
Vehicle: no data
Value: 560 mg/kg bw
Method: other
Year: GLP: no data
Test substance: other TS: Cobratec #99 (benzotriazole); purity >99%
Method: 5 rats/sex/dose, single application of 4 dose levels, post exposure observation time: 14 d
Remark: 398 mg/kg; mortality: 0/10; 502 mg/kg, mortality: 4/10; 632 mg/kg bw, mortality: 7/10; 795 mg/kg, mortality: 10/10
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
04-DEC-2001 (23)

Type: LD50
Species: rat
Strain: other: Greenacres strain
Sex: male
Number of Animals: 5
Vehicle: other: corn oil
Value: 909 mg/kg bw
Method: other
Year: GLP: no data
Test substance: other TS: benzotriazole; purity not noted
Method: The test substance was administered by stomach tube to six groups of 5 male albino rats (weight range 305 - 370 g). The sample was administered in corn oil as a 10% or 50% wt/vol suspension. (Dosage levels of 46.4, 100, 215 mg/kg as 10 % wt/vol; 1000, 150 mg/kg as 50% wt/vol)

Food was withheld for 18 hrs prior to dosing, following which food and water was supplied ad libitum. All animals observed several times during day of dosing for gross signs of systemic toxicity and mortality and daily thereafter for 14 days. Gross autopsies were done on all animals. Statistical analysis of mortality data was done by "moving average" method (Weil, CS. Biometrics. 8:249. 1952)
Result: LD 50 = 909 mg/kg bw (95% conf. limit = 546 - 1510 mg/kg)

Time of death	Dose (mg/kg)					
	46.4	100	215	464	1000	2150
1 hr	0/5	0/5	0/5	0/5	0/5	1/5
2 hr	0/5	0/5	0/5	0/5	1/5	2/5

4 hr	0/5	0/5	0/5	0/5	3/5	2/5
24 hr	0/5	0/5	0/5	0/5	4/5	4/5
2 days	0/5	0/5	0/5	0/5	4/5	4/5
3 days	0/5	0/5	0/5	0/5	4/5	4/5
4 days	0/5	0/5	0/5	0/5	4/5	4/5
5 days	0/5	0/5	0/5	0/5	4/5	4/5
6 days	0/5	0/5	0/5	0/5	4/5	4/5
7-14 days	0/5	0/5	0/5	0/5	4/5	4/5

Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
04-DEC-2001 (24)

Type: LD50
Species: rat
Strain: Sprague-Dawley
Sex: male/female
Number of Animals: 10
Vehicle:
Value: 720 mg/kg bw
Method: other
Year: GLP: no data
Test substance: other TS: benzotriazole residue (sample 81469-B); purity not noted
Method: Five male and five female rats/group were given a single oral dose via blunt tipped canula. Doses levels were 316, 632, 892, 1260 mg/kg. Animals were observed for toxicity and mortality for 14 days. All rats were subjected to a macroscopic examination of the viscera at necropsy.
Remark: The LD50 value was calculated according to Litchfield and Wilcoxon, 1949.
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
04-DEC-2001 (25)

5.1.2 Acute Inhalation Toxicity

Type: LC50
Species: rat
Strain: Sprague-Dawley
Sex: male/female
Number of Animals: 10
Vehicle: other: as a dust
Exposure time: 4 hour(s)
Value: > 1.5 mg/l
Method: other
Year: GLP: no data
Test substance: other TS: benzotriazole; purity not noted
Method: The exposure was conducted for 4 hours at a target level of 2.5 mg/l. Exposure levels were determined by gravimetric

analysis during each hour of exposure. Particle size of the aerosiolized dust was determined using a cascade impactor.

BT was administered via inhalation as a dust, by whole body exposure. Physical observations for abnormal signs were conducted on all animals as a group at 15 minute intervals during the first hour of exposure, and hourly for the remainder of the exposure. All animals received detailed physical observations prior to exposure and upon removal from the chamber, hourly for two hours post exposure, and daily for the 14 day post-exposure period. All animals were sacrificed and complete postmortem examinaitions were performed.

Result: All animals survived the exposure and the 14-day post-exposure observation period. Signs of treatment included slight labored breathing and/or nasal discharge during the exposure or the first week following exposure. These symptoms abated during the second post-exposure week. Slight decreases in weight were observed on the day after exposure with a recovery thereafter. Postmortem examinations were unremarkable.

The mean gravimetric exposure concentration for the 4-hour exposure was determined to be 1.5 mg/l (considered to be the maximum attainable concentration).
**1.5 mg/l for 4 hours is considered equivalent to 6.0 mg/l for 1 hour

Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment

Flag: Critical study for SIDS endpoint

04-DEC-2001 (26)

Type: LC50
Species: rat
Strain:
Sex: male
Number of Animals: 10
Vehicle:
Exposure time: 3 hour(s)
Value: 1.91 mg/l
Method: other
Year: GLP: no data
Test substance: other TS: benzotriazole; purity not noted

Method: Five groups of ten male albino rats were exposed for 3 hours to different concentrations of benzotriazole as a fine aerosol.

Result: The LC50 was determined to be 1.91 mg/l (95% conf. limits = 1.59 - 2.29 mg/l)

Animals which survived the exposure were generally in very good health one-two days post exposure. The primary effect appeared to be pulmonary irritation which resulted intra-tracheal edema and a hemorrhagic type response in the lungs.

Reliability: (2) valid with restrictions

Meets generally accepted scientific standards, well documented and acceptable for assessment

04-DEC-2001 (27)

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rabbit
Strain:
Sex: male/female
Number of Animals: 4
Vehicle: physiol. saline
Value: > 10000 mg/kg bw

Method: EPA OTS 798.1100
Year: GLP: no data
Test substance: other TS: BT-D (benzotriazole) sample no. SD-7413; purity not noted
Method: Dosage levels of 1000, 2150, 4640, 10000 mg/kg bw were applied to intact (2 animals/group) or abraded (2 animals/group) of male and female albino rabbits and occluded for 24 hours. Animals were observed for 14 days post exposure.
Result: No mortalities occurred at any dosage level. With the exception of purulent nasal discharge noted in occasional rabbits, all animals generally exhibited normal appearance and behavior throughout the study.
Reliability: (2) valid with restrictions
Guideline study
Flag: Critical study for SIDS endpoint
04-DEC-2001 (28)

Type: LD50
Species: rat
Strain: no data
Sex: male/female
Number of Animals:
Vehicle: no data
Value: > 2000 mg/kg bw
Method:
Year: 1984 GLP: no data
Test substance: other TS: benzotriazole; purity not noted
Method: other: acute dermal application and a 14 day post-treatment observation period (no further information)
Remark: Symptoms: Dyspnea, exophthalmus, ruffled fur and abnormal body position are symtoms commonly seen during observation time following administration of substances by gavage.
No other symptoms which could be related to the treatment, especially no cutaneous changes, were observed.
24-MAY-2001 (29)

Type: LD50
Species: rabbit
Strain:
Sex:
Number of
Animals: 10
Vehicle:
Value: > 2000 ml/kg bw
Method: other
Year: GLP:
Test substance: other TS: Cobratec 99 (BT) Sample no. 6023; purity >99%
Method: Cobratec 99 was tested for Acute Dermal Toxicity in 10 rabbits at 2000 mg/kg
Result: According to the code of Federal Regulations, the substance is not toxic.
04-DEC-2001 (30)

5.1.4 Acute Toxicity, other Routes

Type: LD50
Species: mouse
Strain:
Sex:
Number of
Animals:
Vehicle:
Route of admin.: i.p.
Value: 1000 mg/kg bw
Method:
Year: GLP: no data
Test substance:
02-OCT-2000 (7)

Type: LD50
Species: mouse
Strain:
Sex:
Number of
Animals:
Vehicle:
Route of admin.: i.v.
Value: 238 mg/kg bw
Method:
Year: GLP: no data
Test substance:
02-OCT-2000 (7)

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result: not irritating
EC classificat.:
Method:
Year: GLP:
Test substance: as prescribed by 1.1 - 1.4
Remark: Exposure period: 4 hour
04-DEC-2001 (13)

5.2.2 Eye Irritation

Species: rabbit
Concentration: undiluted
Dose: 100 other: mg
Exposure Time: 72 hour(s)
Comment: not rinsed
Number of
Animals:
Result: highly irritating
EC classificat.:
Method: Draize Test
Year: GLP: no data
Test substance: other TS: BT-D (benzotriazole) sample no. SD-7413 (Sherwin Williams Co.); purity not noted
Result: Irritative effects included moderate or marked conjunctivitis and corneal opacity, mild iritis, and conjunctival blanching in each rabbit. These signs remained relatively unchanged throughout the 72 hour observation period.
04-DEC-2001 (28) (2)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of
Animals:
Result: slightly irritating
EC classificat.:
Method:
Year: GLP:
Test substance: as prescribed by 1.1 - 1.4
04-DEC-2001 (13)

5.3 Sensitization

Type: Guinea pig maximization test
Species: guinea pig
Number of Animals:
Vehicle:
Result: not sensitizing
Classification:
Method: OECD Guide-line 406 "Skin Sensitization"
Year: GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Reliability: (1) valid without restriction
Guideline study
04-DEC-2001 (13)

5.4 Repeated Dose Toxicity

Species: rat Sex: male/female
Strain: Fischer 344
Route of admin.: oral feed
Exposure period: 78 weeks
Frequency of treatment: daily
Post. obs. period: 26-27 weeks
Doses: 6,700 and 12,100 ppm
Control Group: yes, concurrent no treatment
Method: other: EPA OTS 798.3300
Year: GLP: no data
Test substance: other TS: 1H-benzotriazole; purity > 99%
Method: Groups of 50 Fisher 344 rats of each sex were administered 1H-benzotriazole at one of two time-weighted average doses, either 6,700 or 12,100 ppm for 78 weeks. Except for five control and five high-dose rats of each sex, which were killed at week 78, all animals surviving at that time were observed for an additional 26-27 weeks. Controls consisted of groups of 50 untreated rats of each sex and were observed for 105-106 weeks. All rats surviving to week 104-106 were sacrificed and examined for tumors.
Remark: no clinical symptoms; no influence on mortality
Reliability: (1) valid without restriction
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
26-DEC-2001 (31)

Species: mouse Sex: male/female
Strain: B6C3F1
Route of admin.: oral feed
Exposure period: 104 weeks
Frequency of treatment: daily
Post. obs. period: 2 weeks
Doses: 11,700 and 23,500 ppm
Control Group: yes, concurrent no treatment
Method: other: EPA OTS 798.3300
Year: GLP: no data
Test substance: other TS: 1H-benzotriazole; purity > 99%
Method: Groups of 50 B6C3F1 mice of each sex were administered 1H-benzotriazole at one of two time-weighted average doses, either 11,700 or 23,500 ppm for 104 weeks, then observed for an additional 2 weeks. Controls consisted of groups of 50 untreated mice of each sex and were observed for 109 weeks. All mice surviving to week 106-109 were sacrificed and examined for tumors.
Remark: no clinical symptoms; no influence on mortality
Reliability: (1) valid without restriction
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
26-DEC-2001 (31)

5.5 Genetic Toxicity 'in Vitro'

Type: HGPRT assay
System of testing: CHO cells
Concentration: without: 150, 300, 400, 500, 600, 800, 1000 µg/ml; with: 50, 100, 200, 350, 500, 700, 1000 µg/ml
Cytotoxic Conc.: without: 1000 µg/ml rel. survival: 82.4 % with: 500 µg/ml_ 19.1 %, 1000 µg/ml: 0.0 %
Metabolic activation: with and without
Result: negative
Method: OECD Guide-line 476 "Genetic Toxicology: In vitro Mammalian Cell Gene Mutation Tests"
Year: 1987 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Reliability: (1) valid without restriction
GLP Guideline study
Flag: Critical study for SIDS endpoint
04-DEC-2001 (32)

Type: Ames test
System of testing: Salmonella typhimurium
Concentration:
Cytotoxic Conc.: no data
Metabolic activation: no data
Result: positive
Method:
Year: GLP: no data
Test substance:
04-DEC-2001 (33) (34)

5.6 Genetic Toxicity 'in Vivo'

Type: Micronucleus assay
Species: mouse Sex:
Strain: NMRI
Route of admin.: gavage
Exposure period: once
Doses: 0, 800 mg/kg bw
Result: negative
Method: OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"
Year: 1988 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Reliability: (1) valid without restriction
GLP Guideline study
Flag: Critical study for SIDS endpoint
04-DEC-2001 (35)

5.7 Carcinogenicity

Species: rat Sex: male/female
Strain: Fischer 344
Route of admin.: oral feed
Exposure period: 78 weeks
Frequency of treatment: continuous
Post. obs. period: 26-27 weeks
Doses: 0, 6700, 12100 ppm
Result: negative
Control Group: yes, concurrent no treatment
Method: EPA OTS 798.3300
Year: GLP: no data
Test substance: other TS: 1H-benzotriazole; purity > 99%
Remark: In male rats, neoplastic nodules of the liver occurred at a statistically significant incidence in the high-dose group but the incidence in historic laboratory controls varies from 0-11%; therefore these tumors cannot clearly be associated with test sample administration.
In female rats, incidence of endometrial stromal polyps was significant in the low-dose group, but not significant in the

high-dose group; therefore cannot clearly be associated with test sample administration.
Reliability: (1) valid without restriction
GLP Guideline study
26-DEC-2001 (31)

Species: mouse Sex: male/female
Strain: B6C3F1
Route of admin.: oral feed
Exposure period: 104 weeks
Frequency of treatment: continuous
Post. obs. period: 106 weeks
Doses: 0, 11700, 23500 ppm
Result: negative
Control Group: yes, concurrent no treatment
Method: EPA OTS 798.3300
Year: GLP: no data
Test substance: other TS: 1H-benzotriazole; purity > 99%
Remark: In female mice, incidence of alveolar/bronchiolar carcinomas was statisticallly significant in the low-dose group, but not significant in the high-dose group; therefore occurrence of this tumor cannot clearly be associated with test sample administration.
Reliability: (1) valid without restriction
GLP Guideline study
26-DEC-2001 (31)

Species: Sex:
Strain:
Route of admin.:
Exposure period:
Frequency of treatment:
Post. obs. period:
Doses:
Result:
Control Group:
Method: other: In vitro-Test
Year: GLP:
Test substance:
Remark: Test with Rat Embryo cells;
Result: positive
Source: Bayer AG Leverkusen
26-DEC-2001 (36)

5.8 Toxicity to Reproduction

Type: other
Species: rat Sex: male/female
Strain: Fischer 344
Route of admin.: oral feed
Exposure Period: 78 weeks
Frequency of treatment: continuous
Duration of test: 105 weeks
Doses: 0, 6.700, 12.100 mg/kg bw
Control Group: yes, concurrent no treatment
NOAEL Parental: > 12100 ppm
Method: other: EPA OTS 798.3300
Year: GLP: no data
Test substance: other TS: 1H-benzotriazole; purity > 99%
Remark: The 78 week oral study of 1H-benzotriazole in Fischer 344 rats did not find any evidence of dose-related pathology in the reproductive organs: prostate/testis/epididymis of males and uterus/ovaries of females. Findings, not significantly different from controls, included acute inflammation of the prostate, hyperplasia of the testis, acute inflammation, hydrometra, and hyperplasia of the uterus, inflammation and cyst formation of the ovaries.
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
26-DEC-2001 (31)

Type: other
Species: mouse Sex: male/female
Strain: B6C3F1
Route of admin.: oral feed
Exposure Period: 104 weeks
Frequency of treatment: continuous
Duration of test: 106 weeks
Doses: 0, 11700, 23500 ppm
Control Group: yes, concurrent no treatment
NOAEL Parental: > 23500 ppm
Method: other: EPA OTS 798.3300
Year: GLP: no data
Test substance: other TS: 1H-benzotriazole; purity > 99%
Remark: The 104 week oral study of 1H-benzotriazole in mice did not find any evidence of pathology in the reproductive organs: prostate/testis/epididymis of males and uterus/ovaries of females. Findings, not significantly different from controls, included hyperplasia of the testis, hydrometra and cystic hyperplasia of the uterus, and cyst formation of the ovaries.
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint

26-DEC-2001 (31)

5.9 Developmental Toxicity/Teratogenicity
-

5.10 Other Relevant Information

Type: other
Remark: Extremely strong reaktion at nearly 160 degree C
Source: Bayer AG Leverkusen
28-JAN-1994

5.11 Experience with Human Exposure
-

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(18) Bayer report 248 A/91 D; 1991-07-29

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(27) Huntingdon Research Center. Project No. 745-080. August 8, 1974.

(28) Hill Top Research, Inc. Report T-413. October 29, 1969

(29) Ciba-Geigy Corp., Toxicologiy studies with benzotriazole in rats, rabbits, Chinese Hamsters, Zebra Fish and guinea pigs. OTS0510543-2 6/09/87

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(33) Dunkel, v.c.; Simmon, V.F. in: IARC Publication vol. 27 (1980), S. 283-302

(34) Zeiger, Errol in: Cancer Research 47 (1987), S. 1287-1296 (zitiert in : Ashby, John; Tennart, Raymond in: Mutation Research 204 (1988), S. 17-115)

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7.1 End Point Summary

-

7.2 Hazard Summary

-

7.3 Risk Assessment

-

I U C L I D

D a t a S e t

Existing Chemical	ID: 29385-43-1
CAS No.	29385-43-1
EINECS Name	methyl-1H-benzotriazole
EINECS No.	249-596-6
Molecular Weight	133.2
Molecular Formula	C7H7N3

Producer Related Part
  Company:
  Creation date: 28-MAR-2000

Substance Related Part
  Company:
  Creation date: 28-MAR-2000

Memo: SOCMA, Benzotriazoles Coalition

Printing date: 05-DEC-2001
Revision date:
Date of last Update: 05-DEC-2001

Number of Pages: 31

Chapter (profile): Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile): Reliability: without reliability, 1, 2, 3, 4
Flags (profile): Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 OECD and Company Information

Type: lead organisation
Name: Synthetic Organic Chemical Manufacturers Association (SOCMA), Benzotriazoles Coalition
Street: 1850 M Street N.W., Suite 700
Town: 20036 Washington, D.C.
Country: United States
Phone: (202) 721-4100
Telefax: (202) 296-8120

05-DEC-2001

Type: cooperating company
Name: Bayer Corporation
Country: United States

05-DEC-2001

Type: cooperating company
Name: PMC Specialties Group, Inc.
Country: United States

05-DEC-2001

1.0.2 Location of Production Site
-

1.0.3 Identity of Recipients
-

1.1 General Substance Information

Substance type: organic
Physical status: solid
Purity: > 98 % w/w
05-DEC-2001

1.1.0 Details on Template
-

1.1.1 Spectra
-

1.2 Synonyms

Cobratec TT 100
05-DEC-2001

Methylbenzotriazole
05-DEC-2001

Preventol CI 7-100
05-DEC-2001

Tolyl triazole
05-DEC-2001

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
-

1.9 Source of Exposure
-

1.10.1 Recommendations/Precautionary Measures
-

1.10.2 Emergency Measures
-

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: 76 - 87 degree C
Method: other: Data from Handbook or collection of data
GLP: no data
Testsubstance: other TS: methyl-1H-benzotriazole; purity not noted
Reliability: (2) valid with restrictions
Data from Handbook or collection of data
Flag: Critical study for SIDS endpoint
05-DEC-2001 (1)

Value: 82 - 88 degree C
Testsubstance: as prescribed by 1.1 - 1.4
05-DEC-2001 (2)

2.2 Boiling Point

Value: 160 degree C at 2.67 hPa
Method: other: Data from Handbook or collection of data
GLP: no data
Testsubstance: other TS: methyl-1H-benzotriazole; purity not noted
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
05-DEC-2001 (1)

Value: > 200 degree C
Testsubstance: as prescribed by 1.1 - 1.4
05-DEC-2001 (2)

Value: > 300 degree C
Testsubstance: other TS: methyl-1H-benzotriazole; purity >99%
05-DEC-2001 (3)

2.3 Density

Type: density
Value: 1.13 g/cm3 at 100 degree C
Testsubstance: as prescribed by 1.1 - 1.4
Flag: Critical study for SIDS endpoint
05-DEC-2001 (2)

Type: bulk density
Value: 550 kg/m3
Testsubstance: as prescribed by 1.1 - 1.4
05-DEC-2001 (4)

2.3.1 Granulometry

-

2.4 Vapour Pressure

Value: .04 hPa at 50 degree C
Method: other (measured): Data from Handbook or collection of data
GLP: no data
Testsubstance: other TS: methyl-1H-benzotriazole; purity not noted
Reliability: (2) valid with restrictions
Data from Handbook or collection of data
Flag: Critical study for SIDS endpoint
05-DEC-2001 (1)

Value: .000277 hPa at 25 degree C
Method: other (calculated): MPBPWIN (v1.31)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Result: Vapor Pressure Estimations (25 deg C):
(Using BP: 311.65 deg C (estimated))
(Using MP: 97.46 deg C (estimated))
VP: 0.000147 mm Hg (Antoine Method)
VP: 0.000208 mm Hg (Modified Grain Method)
VP: 0.000385 mm Hg (Mackay Method)
Selected VP: 0.000208 mm Hg (Modified Grain Method)
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
05-DEC-2001 (5)

Value: .00001 hPa at 25 degree C
GLP: no data
Testsubstance: as prescribed by 1.1 - 1.4
05-DEC-2001 (2)

Value: .04 hPa at 20 degree C
Testsubstance: other TS: methyl-1H-benzotriazole; purity >99%
Remark: estimated at 0.3 mmHg
05-DEC-2001 (3)

2.5 Partition Coefficient

log Pow: 1.71 at 25 degree C
Method: other (calculated): KOWWIN v1.65
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Result: Log Kow(version 1.65 estimate): 1.71

SMILES : Cc1cccc2c1nnn2
CHEM : 1H-Benzotriazole, 4(or 5)-methyl-
MOL FOR: C7 H7 N3
MOL WT : 133.15

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE

```
                   Frag|  1  | -CH3    [aliphatic carbon]    | 0.5473 | 0.5473
                   Frag|  6  |Arom. Carbon                   | 0.2940 | 1.7640
                   Frag|  3  |Arom. Nitrogen [5-member ring] |-0.5262 |-1.5786
                   Factor| 1 | 1,2,3-Triazole correction     | 0.7525 | 0.7525
                   Const |   |  Equation Constant            |        | 0.2290
                  -------+-----+-----------------------------------------+--
                  Log Kow   =   1.7142
Reliability:      (2)  valid with restrictions
                  Accepted calculation method
Flag:             Critical study for SIDS endpoint
05-DEC-2001                                                               (5)

log Pow:          2.1
Method:           other (calculated)
  Year:
   GLP:           no data
Testsubstance:    as prescribed by 1.1 - 1.4
05-DEC-2001                                                               (6)
```

2.6.1 Water Solubility

```
Value:            < .1 g/l at 18 degree C
Method:           other: Data from Handbook or collection of data
   GLP:           no data
Testsubstance:    other TS: methyl-1H-benzotriazole; purity not noted
Reliability:      (2)  valid with restrictions
                  Data from Handbook or collection of data
Flag:             Critical study for SIDS endpoint
05-DEC-2001                                                               (1)

Value:            5 g/l at 20 degree C
Testsubstance:    as prescribed by 1.1 - 1.4
05-DEC-2001                                                               (2)

Value:            .55 vol% at 20 degree C
Testsubstance:    other TS: methyl-1H-benzotriazole; purity >99%
05-DEC-2001                                                               (3)
```

2.6.2 Surface Tension

-

2.7 Flash Point

Value: 180 degree C
Type:
Method: other: DIN 51376
Year:
GLP: no data
Testsubstance: as prescribed by 1.1 - 1.4
Reliability: (1) valid without restriction
Meets National standards method (AFNOR/DIN)
05-DEC-2001 (4)

2.8 Auto Flammability

-

2.9 Flammability

-

2.10 Explosive Properties

-

2.11 Oxidizing Properties

-

2.12 Additional Remarks

-

3.1.1 Photodegradation

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1560000 molecule/cm3
Rate constant: .000000000002746 cm3/(molecule * sec)
Degradation: 50 % after 3.9 day
Method: other (calculated): AOP Program (v1.89)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
05-DEC-2001 (5)

3.1.2 Stability in Water
-

3.1.3 Stability in Soil
-

3.2 Monitoring Data (Environment)
-

3.3.1 Transport between Environmental Compartments

Type: fugacity model level III
Media: other: air - sediment(s) - soil - water
Air (Level I):
Water (Level I):
Soil (Level I):
Biota (L.II/III):
Soil (L.II/III):
Method: other: EPIWIN Level III Fugacity Model
Year: 1999
Result:

Media	Distribution (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	2.77	93.5	1000	5.55e-011
Water	39.3	360	1000	2.61e-012
Soil	57.8	360	1000	5.31e-011
Sediment	0.0934	1.44e+003	0	2.06e-012

Media	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	224	303	7.48	10.1
Water	827	429	27.6	14.3
Soil	1.22e+003	0	40.5	0
Sediment	0.491	0.0204	0.0164	0.000681

Persistence Time: 364 hr

Reaction Time: 482 hr
Advection Time: 1.49e+003 hr
Percent Reacted: 75.6
Percent Advected: 24.4

Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
05-DEC-2001 (5)

3.3.2 Distribution
-

3.4 Mode of Degradation in Actual Use
-

3.5 Biodegradation

Type: aerobic
Inoculum: activated sludge, industrial
Concentration: 2 mg/l related to Test substance
Degradation: 77 % after 28 day
Method: OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
Year: 1988 GLP: no
Test substance: as prescribed by 1.1 - 1.4
Remark: test conc.: 2.4, 8, 24, 80 mg/l
Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint
05-DEC-2001 (6)

Type: aerobic
Inoculum: activated sludge
Concentration: 100 mg/l related to Test substance
Degradation: 4 % after 28 day
Method: other: "Manometric Respiration Test acc. to Directive 79/831/EEC, Annex V, Part C (July 1990)
Year: 1992 GLP: yes
Test substance: other TS: purity 99.9 %
Remark: inoculum adapted for 33d
Reliability: (1) valid without restriction
GLP Guideline study
Flag: Critical study for SIDS endpoint
05-DEC-2001 (6)

3.6 BOD5, COD or BOD5/COD Ratio

Method: other: Microbial Inhibition Test

Method: A series of test chambers containing a readily degradable primary substrate (d-glucose), dilution water, and inoculum were dosed with increasing amounts of Cobratec TT-100 (1 to 150 mg/l). Dilution water and primary subtrate controls were conducted concurrently. The Dissolved Oxygen (DO) within each test chamber was measured after the addition of the test sample. The chambers were incubated in the dark for 3 days at a temperature of 18.9 to 20.6 degree C. The DO within each chamber was measured again after the incubation period.
Result: Inhibition of oxygen was not detected over the range of concentrations tested.
Test substance: other TS: tolyltriazole - Cobratec TT-100; purity not noted
05-DEC-2001 (7)

Method: other: Standard Biological Oxygen Demand Ttest (BOD)

Result: Concentrations as high as 2 mg/l will not exert any effect on a wastewater treatment facility.
Test substance: tolyltriazole; purity not noted
14-MAY-2001 (8)

Remark: ThOD: 1562 mg/g
Source: Bayer AG Leverkusen
06-SEP-1995

3.7 Bioaccumulation
-

3.8 Additional Remarks
-

AQUATIC ORGANISMS

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: 42
LC50: 65
Method: other: "Letale Wirkung beim Zebrabaerbling - Brachydanio rerio" (LC 0, LC 50, LC 100; 48-96 Stunden)
Verfahrensvorschlag Umweltbundesamt (Stand: Mai 1984)
Year: 1984 GLP: no
Test substance: as prescribed by 1.1 - 1.4
Reliability: (1) valid without restriction
Meets National standards method (AFNOR/DIN)
Flag: Critical study for SIDS endpoint
05-DEC-2001 (9)

Type:
Species: Lepomis macrochirus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no data
LC50: 31
Method: other: according to Protocol issued by Pesticide Regulation Division of EPA - January 20, 1971
Year: 1971 GLP: no data
Test substance: other TS: tolyltriazole - Cobratec TT-100; purity >99%
Result:

Concentration	Mortality
25.1 ppm	1/20
28.2 ppm	2/20
31.6 ppm	10/20
35.5 ppm	20/20

The LC50 is determined to be 31 ppm with 95% confidence limits of 29.8 to 32.3 ppm.
Reliability: (1) valid without restriction
Meets National standards method (AFNOR/DIN)
Flag: Critical study for SIDS endpoint
05-DEC-2001 (10)

Type:
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no data
LC50: 25.5
Method: other: according to Protocol issued by Pesticide Regulation Division of EPA - January 20, 1971
Year: 1971 GLP: no data
Test substance: other TS: tolyltriazole - Cobratec TT-100; purity >99%
Result:

	96 hr	48 hr	24 hr
LC1 =	14.20 ppm	14.00 ppm	23.00 ppm
LC50 =	25.50 ppm	29.80 ppm	36.90 ppm
LC99 =	46.00 ppm	62.50 ppm	68.50 ppm

Reliability: (1) valid without restriction
Meets National standards method (AFNOR/DIN)
Flag: Critical study for SIDS endpoint
05-DEC-2001 (11)

Type:
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no data
LC50: 21.4
Method: other: according to Protocol issued by Pesticide Regulation Division of EPA - January 20, 1971
Year: 1971 GLP: no data
Test substance: other TS: tolyltriazole - Cobratec TT-100; purity >99%
Result:

	96 hr	48 hr
LC1 =	9.10 ppm	9.40 ppm
LC50 =	21.40 ppm	38.00 ppm
LC99 =	51.00 ppm	*

Reliability: (1) valid without restriction
Meets National standards method (AFNOR/DIN)
Flag: Critical study for SIDS endpoint
05-DEC-2001 (12)

4.2 Acute Toxicity to Aquatic Invertebrates

Type:
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring:
EC0: 16
EC100: 78.4
geom. mean : 35.4
Method: other: Directive 67/548/EEC, (C.2) "Acute Toxicity for Daphnia" (29.12.1992)
Year: 1994 GLP: no
Test substance: other TS: methyl-1H-benzotriazole; purity 99.9 %
Remark: analyt. monit.: TOC
Source: Bayer AG Leverkusen
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
05-DEC-2001

Type:
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring:
LC50 : 73.7
Method:
Year: GLP:
Test substance: other TS: methyl-1H-benzotriazole; purity >99%
05-DEC-2001 (3)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Scenedesmus subspicatus (Algae)
Endpoint: growth rate
Exposure period: 72 hour(s)
Unit: mg/l Analytical monitoring:
EC50: 62
Method: other: "Algal Inhibition Test" (c.3), Directive 67/548/EEC (29.12.92)
Year: 1992 GLP: yes
Test substance: other TS: methyl-1H-benzotriazole; purity 99.9 %
Remark: Arithm. mean of analytically determined values:
Biomass
EC10: 10 mg/l
EC50: 32 mg/l
Growth rate
EC10: 24 mg/l
EC50: 62 mg/l
Dunnett-Test
NOEC: 7.5 mg/l
LOEC: 10.0 mg/l
Prior to the test, the TS was crushed with a pistil, weighed into water and treated in an ultrasonic bath for 30 minutes. All test results are related to TOC; 1 mg/l TOC equals 1.6 mg/l TS.

Reliability: (1) valid without restriction
GLP Guideline study
Flag: Critical study for SIDS endpoint
05-DEC-2001 (13)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type: aquatic
Species: activated sludge
Exposure period: 3 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 330
Method: other: E 3002: The Assessment of the Possible Inhibitory Effect of Dyestuffs on Aerobic Waste Water Bacteria. Experience with a Screening Test. Brown, D.; Hitz, H.R.; Schaefer, L.: Chemosphere 10 (3), 245-261 (1981)
Year: 1982 GLP: no
Test substance:
05-DEC-2001 (6)

Type: aquatic
Species: Pseudomonas putida (Bacteria)
Exposure period: 30 minute(s)
Unit: mg/l Analytical monitoring: no
EC0: 31.25
Method: other: Bewertung toxischer Wasserinhaltsstoffe aus ihrer Inhibitorwirkung auf die Substratoxydation von Pseudomonas Stamm Berlin mit Hilfe polarographischer Sauerstoffmessungen. Robra, K.H.: gwf wasser/abwasser 117 (2), 80-86 (1976)
Year: 1982 GLP: no
Test substance:
05-DEC-2001 (6)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

-

4.5.2 Chronic Toxicity to Aquatic Invertebrates

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Species:          Daphnia magna  (Crustacea)
Endpoint:
Exposure period:  21 day
Unit:             mg/l                   Analytical monitoring:
Method:           OECD Guide-line 202, part 2  "Daphnia sp., Reproduction Test"
  Year:           1995                                      GLP: yes
Test substance:   other TS: methyl-1H-benzotriazole; purity 99.9 %
Remark:           Arithm. mean of analytically determined values:
                  EC50 (Immobilisation): > 37.6 mg/l TS
                                         > 23.5 mg/l TOC
                  EC50 (Reproduction):   > 18.4 < 37.6 mg/l TS
                                         > 11.5 < 23.5 mg/l TOC
                  NOEC (Reproduction):     18.4 mg/l TS
                                           11.5 mg/l TOC
                  LOEC (Reproduction):     37.6 mg/l TS
                                           23.5 mg/l TOC
                  Before starting the test, the TS was crushed with a pistil.
                  To produce the stock solution, the TS was weighed into
                  water, treated in an ultrasonic bath for 1 hour and
                  subsequently stirred on a magnetic stirrer for 24 hours.
Reliability:      (1)  valid without restriction
                  GLP Guideline study
05-DEC-2001                                                                (6)
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TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms

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4.6.2 Toxicity to Terrestrial Plants

-

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 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Strain:
Sex: male
Number of Animals: 5
Vehicle: other: corn oil
Value: 1470
Method:
Year: GLP: no data
Test substance: other TS: methylbenzotriazole; purity >99%
Method: The test substance was administered orally by stomach tube to six groups of 5 male albino rats (weight range 247 - 345 g). The sample was administered in corn oil as a 10% or 50% wt/vol suspension. (Dosage levels of 46.4, 100, 215 mg/kg as 10 % wt/vol; 464, 1000, 2150 mg/kg as 50% wt/vol).

Food was withheld for 18 hrs prior to dosing, following which food and water was supplied ad libitum. All animals were observed several times during day of dosing for gross signs of systemic toxicity and mortality and daily thereafter for 14 days. Gross autopsies were done on all animals. Statistical analysis of mortality data was done by "moving average" method (Weil, CS. Biometrics. 8:249. 1952).

Result: LD 50 = 1470 mg/kg bw (95% conf. limit could not be calculated due to "all or none" response.)

Time of death	Dose (mg/kg)					
	46.4	100	215	464	1000	2150
1 hr	0/5	0/5	0/5	0/5	0/5	0/5
2 hr	0/5	0/5	0/5	0/5	0/5	0/5
4 hr	0/5	0/5	0/5	0/5	0/5	0/5
24 hr	0/5	0/5	0/5	0/5	0/5	5/5
2 days	0/5	0/5	0/5	0/5	0/5	5/5
3 days	0/5	0/5	0/5	0/5	0/5	5/5
4 days	0/5	0/5	0/5	0/5	0/5	5/5
5 days	0/5	0/5	0/5	0/5	0/5	5/5
6 days	0/5	0/5	0/5	0/5	0/5	5/5
7-14 days	0/5	0/5	0/5	0/5	0/5	5/5

Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
05-DEC-2001 (14)

Type: LD50
Species: rat
Strain: other: FDRL strain
Sex: male/female
Number of Animals: 5
Vehicle: CMC
Value: 1830 mg/kg bw
Method: other: as recommended in "Appraisal of Safety of Chemicals in Food, Drugs, and Cosmetics" Association of Food and Drug Officials of the US. 1959
Year: 1959 GLP: no data
Test substance: other TS: tolutriazole, OLIN 58734; purity not noted
Result: LD 50 = 1830 mg/kg bw (95% conf. limit = 1200-2810 mg/kg)

MORTALITY DATA

Time of death	Dose (mg/kg)				
	500	1000	2000	4000	8000
5 min	0/5	0/5	0/5	5/5	5/5
1/2 -3 hr	0/5	0/5	3/5	5/5	5/5
7 days	1/5	0/5	3/5	5/5	5/5

Observations:
500 mg/kg - CNS depression, shallow breathing, nasal bleeding
1000 mg/kg - CNS depression
2000 mg/kg - CNS depression, shallow breathing
4000 mg/kg - CNS depression, shallow breathing, eyes tearing
8000 mg/kg - CNS depression, salivation
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
05-DEC-2001 (15)

Type: LD50
Species: rat
Strain:
Sex: male/female
Number of Animals: 10
Vehicle:
Value: 1625 ml/kg bw
Method: EPA OTS 798.1175
Year: GLP: no data
Test substance: other TS: tolyltriazole residue; purity not noted
Reliability: (2) valid with restrictions
Meets National standards method (AFNOR/DIN)
05-DEC-2001 (16)

Type: LD50
Species: rat
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: 675
Method:
Year: GLP:
Test substance: other TS: tolyltriazole - Cobratec TT-100; purity >99%
05-DEC-2001 (17)

Type: LD50
Species: rat
Strain: Wistar
Sex: male/female
Number of
Animals: 10/dose
Vehicle: DMSO
Value: 720 mg/kg bw
Method:
Year: GLP: no data
Test substance: as prescribed by 1.1 - 1.4
05-DEC-2001 (6)

Type: LD50
Species: rat
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: 675 mg/kg bw
Method:
Year: GLP:
Test substance: other TS: methyl-1H-benzotriazole; purity not noted
05-DEC-2001 (1) (3)

Type: LD50
Species: rat
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: 1600 mg/kg bw
Method:
Year: GLP:
Test substance: other TS: methyl-1H-benzotriazole; purity not noted
05-DEC-2001 (1)

5.1.2 Acute Inhalation Toxicity

Type: other: Acute Inhalation Toxicity
Species: rat
Strain: Sprague-Dawley
Sex: male/female
Number of Animals: 20
Vehicle:
Exposure time: 1 hour(s)
Value: > 1.73 mg/l
Method:
Year: GLP: no data
Test substance: other TS: tolyltriazole; purity not noted
Method: Ten male and 10 female Sprague-Dawley rats were exposed for one hour to an aerosol of tolyltriazole at actual concentration of 1.73 +/- 0.67 mg/l, and EAD of 0.35 micron, a geomeetric standard deviation of 2.62 ug/l.
The animals were observed for toxicity and mortality during the exposure and daily for a 14 day post-exposure period. All animals were necropsied and all organs observed for gross abnormalities.
Result: No deaths ocurred during the 14 day post-exposure period. No significant pharmacologic or toxicologic signs were noted.
All animals appeared in good health post-exposure and gained weight normally. The primary effect observed on necropsy was pulmonary irritation.
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
05-DEC-2001 (18)

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rabbit
Strain:
Sex: male/female
Number of Animals: 4
Vehicle: water
Value: > 4000 mg/kg bw
Method: other: as recommended in "Appraisal of Safety of Chemicals in Food, Drugs, and Cosmetics" Association of Food and Drug Officials of the US. 1959
Year: 1959 GLP: no data
Test substance: other TS: tolutriazole, OLIN 58734; purity not noted
Result: No deaths ocurred at any dose level in 14 days. No noteworthy findings were observed.

Primary irritation scores -
500 mg/kg = 1.4
1000 mg/kg = 1.5

2000 mg/kg = 1.1
4000 mg/kg = 1.4
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
05-DEC-2001 (15)

Type: LD50
Species: rabbit
Strain:
Sex:
Number of Animals: 10
Vehicle:
Value: > 2000 mg/kg bw
Method: other: Huntingdon Reserach Center protocol
Year: GLP: no data
Test substance: other TS: Cobratec TT-100 (tolyltriazole); purity not noted
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
05-DEC-2001 (19)

5.1.4 Acute Toxicity, other Routes

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.p.
Value:
Method:
Year: GLP:
Test substance:
Remark: male: 172 mg/kg
female: 237 mg/kg
05-DEC-2001 (6)

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result: not irritating
EC classificat.:
Method:
Year: GLP:
Test substance:
Remark: exposure time: 4 hours
05-DEC-2001 (6)

5.2.2 Eye Irritation

Species: rabbit
Concentration: undiluted
Dose: 10 other: mg
Exposure Time:
Comment: not rinsed
Number of
Animals: 6
Result: slightly irritating
EC classificat.:
Method: other: as recommended in "Appraisal of Safety of Chemicals in Food, Drugs, and Cosmetics" Association of Food and Drug Officials of the US. 1959. p. 46
Year: 1959 GLP: no data
Test substance: other TS: tolutriazole, OLIN 58734; purity not noted
Result: Irritation Score:

Rabbit No. & sex	day 1	day 2	day 3
2201M	6	2	0
2202M	23	2	0
2203M	45	24	24
2204F	4	0	0
2205F	20	12	2
2206F	10	4	0

(maximum irritation score = 110)

Reliability: (1) valid without restriction
Meets generally accepted scientific standards, well documented and acceptable for assessment
05-DEC-2001 (15)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: not irritating
EC classificat.:
Method:
Year: GLP:
Test substance:
05-DEC-2001 (6)

5.3 Sensitization

Type: Guinea pig maximization test
Species: guinea pig
Number of Animals:
Vehicle:
Result: not sensitizing
Classification:
Method:
Year: GLP:
Test substance:
05-DEC-2001 (6)

5.4 Repeated Dose Toxicity

Species: rat Sex:
Strain: Wistar
Route of admin.: gavage
Exposure period: 29 d
Frequency of treatment: daily
Post. obs. period:
Doses: 0, 50, 150, 450 mg/kg
Control Group: yes, concurrent vehicle
NOAEL: 150 mg/kg
Method:
Year: GLP:
Test substance: as prescribed by 1.1 - 1.4
Result: In the highest dose group signs of mild apathy could be observed. Haematological and histopathological results were within the reference ranges.
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
05-DEC-2001 (20)

Species: rat Sex:
Strain:
Route of admin.: gavage
Exposure period: 9 d
Frequency of treatment: 1/d
Post. obs. period:
Doses: 0, 100, 500 mg/kg
Control Group:
Method:
Year: GLP:
Test substance:
Remark: Lethargy and respiratory difficulties after each dose; no macroscopic noticeable changes to organs and tissues. [Sedation und Atembeschwerden nach jeder Applikation der naechsten Dosis; krinr makroskopischen Auffaelligkeiten an Organen und Geweben]
Source: Bayer AG Leverkusen
05-DEC-2001 (6)

5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: Salmonella typhimurium TA-1535, 1537, 1538, 98, 100
Concentration: 0.80, 0.4, 2, 10 mg/plate
Cytotoxic Conc.: 10 mg/ plate
Metabolic activation: with and without
Result: negative
Method: EPA OTS 798.5265
Year: GLP: no data
Test substance: other TS: Cobratec TT-100 (tolyltriazole); purity >99%
Remark: Activation system liver homogenate was prepared from Sprague-Dawley adult male rats induced by Arochlor 1254, five days before sacrifice.
Result: The revertant response elicited at the highest concentration indicated a slight elevation of the revertant rate but did not produce a response of at least 2x background and is negated by the toxicity of the compound.
Reliability: (1) valid without restriction
Meets National standards method (AFNOR/DIN)
Flag: Critical study for SIDS endpoint
05-DEC-2001 (21)

Type: DNA damage and repair assay
System of testing: Human embryonic lung fibroblasts (WI-38)
Concentration: 0.8, 8, 40, 80 ug/plate
Cytotoxic Conc.: EC50 = 20 ug/plate as determined by screening cytotoxicity assay
Metabolic activation: without
Result: negative
Method: EPA OTS 798.5550
Year: GLP: no data
Test substance: other TS: Cobratec TT-100 (tolyltriazole); purity >99%
Result: Cobratec TT-100 did not elicit significant 3H-TdR incorporations above control levels at any dose level tested.
Reliability: (1) valid without restriction
Meets National standards method (AFNOR/DIN)
Flag: Critical study for SIDS endpoint
05-DEC-2001 (21)

Type: other: Mouse fibroblast Transformation Assay
System of testing: C3H 10T1/2 mouse embryonic fibroblastic cell line
Concentration: 6, 60, 600 ug/plate
Cytotoxic Conc.: EC50 = 4 ug/plate as determined by screening cytotoxicity assay
Metabolic activation: without
Result: negative
Method:
Year: GLP: no data
Test substance: other TS: Cobratec TT-100 (tolyltriazole); purity not noted
Method: Two sets of 60mm culture dishes are seeded with cells. One set of dishes, 12 replicates per dose, is seeded with 1000 cells. This set is used for the transformation assay. The second set was seeded with 200 cells per dish, 3 replicates/dose, and is utilized for cytotoxicity determinations.

Both sets of cells are treated in an identical manner with solutions of the test material. Following a 24-hour exposure period, the toxicant is washed from all plates and the cells refed with normal growth media. Ten days following the initial seeding, the plates designated for cytotoxicity assay are washed, fixed with methanol, and stained. The clones on all plates are counted and the plating efficiency counted. This plating efficiency is expressed as the number of colonies formed as a percentage of the number of cells seeded.

The transformation plates are incubated for 6 weeks with weekly medium changes. During this time, the clones grow to form a confluent monolayer of cells on the bottom of the plates. At the termination of the incubation period, all remaining plates are washed, fixed, stained and scored for transformed foci.

Type I foci : tightly packed cells
Type II foci : massive piling into opaque multilayers
Type III foci : highly polar, densely stained cells, which form a criss-crossed multilayer

Type II and III are considered to be malignantly transformed. The transformation frequency is calculated as the percentage of cells that give rise to transformed foci corrected for plating efficiency, which is determined by the cytotoxicity assay.

Remark: The C3H 10T1/2 line is a fibroblastic cell line, derived from C3H mouse embryos which are highly sensitive to postconfluence inhibition of cell division. When C3H 10T1/2 cells are exposed to a variety of chemical carcinogens, morphologically transformed foci develop with a frequency that is dose dependent. The foci have been shown to produce fibrosarcomas when injected into syngenic mice. Therefore, the C3H 10T1/2 cell line can be used to assay for chemical carcinogens.

Result: Cobratec TT-100 did not produce significant increases in transformation above control cell population levels. As a positive control, the cells did respond in a dose-dependent manner to the chemical carcinogen dimethylbenzanthracene (DMBA).

05-DEC-2001 (21)

Type: Ames test
System of testing: Salmonella typhimurium TA97, TA98, TA100, TA1535, TA1537
Concentration: 0, 33, 100, 333, 1000, 1666, 3333, 6666 ug/plate
Cytotoxic Conc.: strain TA1535 cytotoxic at 6666 ug/plate
Metabolic activation: with and without
Result:
Method:
Year: GLP: no data
Test substance: other TS: tolyltriazole, CAS#29385-43-1, obtained from Sherwin Williams; purity >99%
Remark: Solvent: DMSO
Metabolic activation: HLI= Aroclor-induced hamster liver S-9
RLI=Aroclor-induced rat liver S-9

Result:

Strain	TA100	TA1535	TA97	TA98
NA	-	-	-	-
5% HLI	?	NT	NT	-
10% HLI	? +w ?	-	-	?
30%HLI	-	NT	NT	-
5% RLI	+	NT	NT	NT
10% RLI	? + ?	-	-	-
30% RLI	+w	NT	NT	NT

- = non-mutagenic
? = questionable mutagenic response

+w = weakly mutagenic
+ = mutagenic
NT = not-tested

05-DEC-2001 (22)

Type: Ames test
System of testing: Salmonella typhimurium
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen

05-DEC-2001 (6)

5.6 Genetic Toxicity 'in Vivo'

Type: Micronucleus assay
Species: mouse Sex: male/female
Strain: other: Bor. NMRRI; manufactor Winkelmann
Route of admin.: oral unspecified
Exposure period: single exposure
Doses: 600 mg/kg
Result: negative
Method: OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"
Year: 1987 GLP: yes
Test substance: other TS: Preventol CI 7-100; purity 99,3 %
Reliability: (1) valid without restriction
GLP Guideline study
Flag: Critical study for SIDS endpoint

05-DEC-2001 (23)

5.7 Carcinogenicity
-

5.8 Toxicity to Reproduction
Remark: The 78 week oral study of 1H-benzotriazole (95-14-7) in Fischer 344 rats and the 104 week oral study of 1H-benzotriazole in B6C3F1 mice did not find any evidence of pathology in the reproductive organs. The organs examined were: prostate/testis/epididymis of males and uterus/ovaries of females.

06-DEC-2001 (24)

5.9 Developmental Toxicity/Teratogenicity
-

5.10 Other Relevant Information
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5.11 Experience with Human Exposure
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(1) NTP Chemical Repository, Catlog ID Number 001439

(2) Safety Data Sheet Bayer AG, 15.06.2000

(3) PMC Specialties Group, Inc., MSDS 12/30/96

(4) Safety Data Sheet Bayer AG, 27.04.1990

(5) Meylan W. and Howard P. (1999) EPIWin Modeling Program. Syracuse Research Corporation. Environmental Science Center, 6225 Running Ridge Road, North Syracuse, NY 13212-2510.

(6) Bayer AG report, 25.04.88

(7) Wildlife International Ltd. Easton, MD. Project No. 373E-105. June 11, 1993

(8) Agatha Corporation. Cincinnati, OH. February 7, 1973

(9) Bayer report. Lab.No. 8503862 - 2418; 1985-09-19

(10) Huntingdon Research Center, New City, NY. Study No. 759-236. September 24, 1975

(11) Huntingdon Research Center, Brookville, MD. Study No. 744-067. October 31, 1974

(12) Huntingdon Research Center, Brookville, MD. Study No. 744-06. December 17, 1974

(13) Bayer report. No 501A / 94 A 1; 1994-09-27

(14) Hill Top Research, Inc. Miamiville, OH. Study No. S-275. August 21, 1968

(15) Food and Drug Research Laboratories. Lab no. 88722. Maspeth, NY. February 2, 1968.

(16) North American Science Associates, Inc. Northwood, OH. Study No. 81-5480. August 28, 1981

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7.1 End Point Summary

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7.2 Hazard Summary

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7.3 Risk Assessment

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