201-13324

COURTNEY M. PRICE
VICE PRESIDENT
CHEMSTAR

American Chemistry Council
Good Chemistry Makes It Possible

November 30, 2001

Via US Mail and e-mail

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

Re: Rubber and Plastic Additives (RAPA) Panel, Consortium No.
HPV Chemical Challenge Program Submission
Benzothiazole-based Thiazoles Category
Category Justification and Testing Rationale

Dear Governor Whitman:

The RAPA Panel of the American Chemistry Council is pleased to submit the subject documents to EPA's HPV Chemical Challenge Program (Program) as our initial test plan for a category covering four of the 39 chemicals RAPA is voluntarily sponsoring in the Program. The RAPA Panel includes the following member companies: Bayer Corporation, Ciba Specialty Chemicals Corporation, Crompton Corporation, Flexsys America L.P., The Goodyear Tire & Rubber Company, The Lubrizol Corporation, Noveon, Inc., R.T. Vanderbilt Company, Inc., and UOP, LLC.

In this submission, please find the *Category Justification and Testing Rationale* for the category *Benzothiazole-based Thiazoles*. Four chemicals in the category are sponsored in the Program, as listed in the following table:

RAPA Panel Benzothiazole-based Thiozole Category Chemicals Sponsored in the US HPV Chemical Challenge Program	
CAS Number	**Compound Name**
95-32-9	Benzothiazole, 2-(morpholinodithio)-
149-30-4	2(3H)-Benzothiazolethione
155-04-4	2(3H)-Benzothiazolethione, zinc salt
2492-26-4	2(3H)-Benzothiazolethione, sodium salt

Responsible Care®

MR-53125

1300 Wilson Boulevard, Arlington, VA 22209 • Tel 703-741-5600 • Fax 703-741-6091 • http://www.americanchemistry.com

Data for two additional chemicals in the category, listed in the table below, are used to support the conclusions reached for the category.

RAPA Panel Benzothiazole-based Thiozole Category Additional Chemicals in the Category	
CAS Number	**Compound Name**
95-16-9	Benzothiozole
120-78-5	Benzothiazole, 2,2'-dithiobis-,

In addition to the *Category Justification and Testing Rationale*, please also find attached robust summaries contained in IUCLID-formatted documents for each of the four sponsored chemicals and the two supporting chemicals in the category.

This submission is also being sent electronically to the following e-mail addresses:

Oppt.ncic@epa.gov
Chem.rtk@epa.gov

If you require additional information, please contact the RAPA Panel's technical contact, Dr. Anne P. LeHuray at (703) 741-5630 or anne_lehuray@americanchemistry.com.

Sincerely yours,

Courtney M. Price
Vice President, CHEMSTAR

Attachments

cc: C. Auer, EPA/OPPT
B. Leczynski, EPA/OPPT
RAPA Panel (without attachments)
S. Russell, ACC (without attachments)

Benzothiazole-based Thiazoles
Category Justification and Testing Rationale

CAS Nos.: **95-32-9; 149-30-4; 155-04-4; 2492-26-4**
(+ SIDS Chemicals 95-16-9 and 120-78-5 for data purposes)

Rubber and Plastic Additives Panel
American Chemistry Council
November, 2001

List of Member Companies in the Rubber and Plastic Additives Panel

The Rubber and Plastic Additives Panel of the American Chemistry Council include the following member companies: Bayer Corporation, Ciba Specialty Chemicals Corporation, Crompton Corporation, Flexsys America L.P., The Goodyear Tire & Rubber Company, The Lubrizol Corporation, Noveon, Inc., R.T. Vanderbilt Company, Inc., and UOP, LLC.

Executive Summary

The American Chemistry Council's Rubber and Plastic Additives Panel (RAPA), and its member companies, hereby submit for review and public comment their test plan for the Benzothiazole-based Thiazoles category of chemicals under the Environmental Protection Agency's High Production Volume (HPV) Chemical Challenge Program.

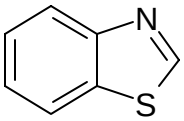
As discussed in the report that follows, Benzothiazole-based thiazoles , which are used primarily as cure- rate accelerators in natural and synthetic rubbers or as chemical intermediates in the manufacture of rubber accelerators, are defined as possessing a benzothiazole backbone [benzene ring + thiazole ring] with various substitutions at the #2 position on the thiazole ring. Their use in the rubber vulcanization process requires stability at high temperatures, low biodegradation, negligible water solubility and low vapor pressure. Non-rubber applications for this category include metal chelation, ore flotation, corrosion inhibition, veterinary drugs and industrial biocide/water treatment for 2-mercapto-benzothiazole and sodium 2-mercaptobenzothiazole.

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 also 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. Existing data for members of this category indicate that they are of moderate concern for aquatic toxicity, low concern as Persistent Organic Pollutants (POP), moderate concern for skin irritation/allergic skin reaction, and low concern for mammalian toxicity and carcinogenicity. In addition, the Food and Drug Administration has approved several food-contact uses for this category of chemicals. We conclude that there is sufficient data on the members of this category for purposes of the HPV Program and no additional testing is recommended.

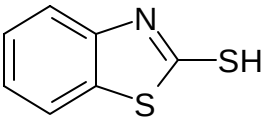
Benzothiazole-based Thiazoles category

As defined by EPA under the HPV Chemical Program, a chemical category is "a group of chemicals whose physico-chemical 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 with specific consideration of animal welfare concerns to minimize the use of animals in the testing of chemicals.

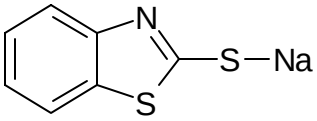
Relying on several factors specified in EPA's guidance document on "Development of Chemical Categories in the HPV Challenge Program,"[1] in which use of chemical categories is encouraged, the following closely related chemicals constitute a chemical category:



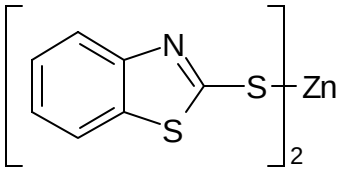
95-16-9
Benzothiazole (BTH)



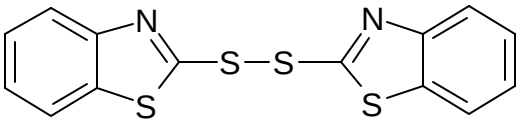
149-30-4
2-Mercaptobenzothiazole (MBT)



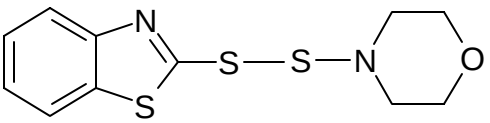
2492-26-4
Sodium 2-mercaptobenzothiazole (NaMBT)



155-04-4
Zinc 2-mercaptobenzothiazole (ZMBT)



120-78-5
Benzothiazole disulfide (MBTS)



95-32-9
Benzothiazole, 2-(4-morpholinyldithio)- (MORFAX)

Figure 1. Chemical structures

[1] US EPA, Office of Pollution Prevention and Toxics. Development of Chemical Categories, Chemical Right-to-Know Initiative. http://www.epa.gov/opptintr/chemrtk/categuid.htm

Structural Similarity

A key factor supporting the classification of these chemicals as a category is their structural similarity. All materials in this category contain the benzothiazole backbone [benzene ring + thiazole ring] with various substitutions on the #2 carbon of the thiazole ring.

Common Precursors

Starting materials and the reaction process are identical for all category members. Aniline, carbon disulfide and sulfur are reacted to form crude 2-mercaptobenzothiazole and benzothiazole. All remaining category members are produced in step-wise batch reactions from this crude 2-Mercaptobenzothiazole.

Common Breakdown Products

2-mercaptobenzothiazole is formed when these compounds undergo hydrolysis and/or dissociation.

Similarity of Physicochemical Properties

The similarity of the physicochemical properties of these materials parallels their structural similarity. All exhibit limited water solubilities, low vapor pressures, high flash points, high boiling points, excellent thermal stability, lack of reactivity, and Log P values at or below 5.

Table 1. Physico-chemical Properties

Chemical **CAS#**	Benzothiazole **95-16-9**	2-Mercapto benzothiazole **149-30-4**	Sodium 2-mercapto benzothiazole **2492-26-4**	Zinc mercapto Benzothiazole **155-04-4**	Benzothiazole 2-(4-morpho linyldithio)- **95-32-9**	Benzothiazole Disulfide **120-78-5**
Molecular Weight:	135.18	167.24	167.24	397.7	284.42	332.38
Melting Point	2°C	181°C	85.8°C (EPI)	233° C (EPI)	173°C (EPI)	180°C
Boiling Point	230°C	decomp above 260°C	301°C (EPI)	544.40°C (EPI)	418.3°C (EPI)	decomp
Relative Density	1.246g/cm3 @20°C	1.42g/cm3 @20°C	1.25g/cm3 @25°C	1.7g/cm3	1.51g/cm3	1.54g/cm3 @25°C
Vapour Pressure	0.13 hPa @20°C	3.0 x10(-6) hPa @25°C	6.0 x10(-4) hPa @25C (EPI)	1.546 x10(-11) hPa @25°C (EPI)	1.16 x10(-7) hPa @25°C (EPI)	5.97 x10(-10) hPa @20°C
Partition Coefficient	2	2.4 (2.86 EPI)	2.4	5.0 (EPI)	1.59 (EPI)	4.5 (4.66 EPI)
Water Solubility	3g/l @20°C	118mg/l @25°C pH 7.0	>500 mg/l @25°C pH12.5	90.9 mg/l @20°C	657.6 mg/l @25°C (EPI)	80 – 96 mg/l @22°C pH 5.0

= Non-sponsored chemicals used for data purposes only

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

Fate and Transport Characteristics

Test data indicate that members of this category are not readily biodegradable when measured by CO_2 evolution, mineralization or hydrolysis, and marginal by indirect photolysis. For purposes of the HPV Program, additional testing is not needed. Testing has shown that, if hydrolysis occurs, the primary hydrolysis product is 2-MBT. Adequate information regarding photodegradation is available, so additional data collection efforts are not necessary. Fugacity modeling has been done for all members of the category and in practice have been shown not to partition to water or air if released into the environment due to their low water solubility and low vapor pressure. (See Table 2)

Toxicological Similarity

Review of existing published and unpublished test data for Benzothiazole-based Thiazoles shows the *aquatic and mammalian toxicity* among the materials within this category are similar. The sodium and zinc salts are expected to immediately dissociate and form mercaptobenzothiazole in an aqueous environment. Studies demonstrate that the salts are less toxic than mercaptobenzothiazole (acute fish toxicity, Daphnia EC50, and acute oral toxicity in rats).

Aquatic Toxicology - Acute

Data on acute fish toxicity, acute invertebrate toxicity, and algal toxicity were reviewed. The Benzothiazole-based Thiazoles range from highly toxic to practically non-toxic. Acute studies on *Pimephales* promelas demonstrate a 96-hour LC_{50} ranging from 11 mg/l (#149-30-4) to greater than 1000 mg/l (#120-78-5). Acute studies on *Daphnia magna* demonstrate a 48-hour EC_{50} ranging from 4.1mg/l (#149-30-4) to greater than solubility range (#120-78-5). Acute studies on Algae demonstrate a 96-hour EC_{50} ranging from 0.25 mg/l (#149-30-4) to greater than solubility range (#120-78-5). Data are available for most chemicals in this category and ECOSAR modeling data is available for the others; therefore sufficient data is available to adequately evaluate the toxicity to aquatic organisms. For purposes of the HPV Program, no additional ecotoxicity toxicity testing is necessary. (See Table 3)

Mammalian Toxicology - Acute

Data on acute mammalian toxicity were reviewed, and the findings indicate a low concern for acute toxicity for all materials. Data are available for most members of the category by the oral and dermal routes of exposure, and inhalation exposure testing has been done on three members of the category, indicating that the category has been well tested for acute mammalian effects. Therefore, for purposes of the HPV Program, no additional acute mammalian toxicity testing is necessary. (See Table 4)

Mammalian Toxicology - Mutagenicity

Data from bacterial reverse mutation assays, *in vitro* and *in vivo* chromosome aberration studies, as well as additional supporting *in vitro* and *in vivo* genetic toxicity studies were reviewed, and the findings indicate a low

concern for mutagenicity. Data are available for all members of the category in the Ames assay. Data are available for all but one chemical for chromosome aberration studies, and these data can be bridged to the other member of the category. There are also carcinogenicity studies available and summarized in the IUCLID documents. Therefore, the category has been adequately tested for mutagenicity for the purposes of the HPV Program, and no additional mutagenicity testing is necessary. (See Table 4)

Mammalian Toxicology – Repeated Dose Toxicity

Data from repeated-dose toxicity studies were reviewed. CAS# 149-30-4 has 28 day, 90 day and chronic studies, which can be bridged to the salts (#155-04-4 and #2492-26-4). There is also a 90 day and chronic study on CAS# 120-78-5. Sufficient data are available to adequately characterize the repeated dose toxicity of this category through bridging to members without test data, such that for purposes of the HPV Program, additional testing is not necessary for these materials. (See Table 4)

Mammalian Toxicology - Reproductive and Developmental Toxicity

There are several adequate reproductive/developmental studies for members of this category. A 2-generation study on CAS# 149-30-4 can be bridged to the salts (#155-04-4 and #2492-26-4). There is also a study on CAS# 120-78-5. Sufficient data are available to adequately characterize the Reproductive and Developmental toxicity of this category through bridging to members without test data. Additional testing will not provide useful and relevant information for this category, therefore for purposes of the HPV Program, testing is not necessary. (See Table 4)

Epidemiology

Two long-term mortality studies have been published on men employed in the production of MBT, MBTS, NaMBT and ZMBT at manufacturing sites in the USA and Europe.
The European study followed 2160 men employed since 1955 and with at least six months exposure to this category of chemicals. The American study followed 1059 employees with a similar work history. There were no statistically significant increases in types of cancer, cancer rates or cancer deaths that could be attributed to chemicals from this category.

Conclusion

Based upon the data reviewed in the report, the reaction routes, the precursors, the physicochemical and toxicological properties of the proposed Benzothiazole-based Thiazoles category members are similar and follow a regular pattern as a result of that structural similarity. Therefore, the EPA's definition of a chemical category has been met.

Test Plan

The test plan for the Benzothiazole-based Thiazoles category was developed giving careful consideration to the number of animals that would be required for any tests that are not available for certain members of the category and whether these additional tests would provide useful and relevant information. We conclude that there is sufficient data on the members of this category for the purposes of the HPV Program, and no additional testing is recommended. (See Table 5)

Table 2. Matrix of Available and Adequate Data on Benzothiazole-based Thiazoles Category
Environmental Fate

Endpoint	Benzothiazole 95-16-9 (SIDS)	2-Mercapto benzothiazole 149-30-4	Sodium 2-mercapto benzothiazole 2492-26-4	Zinc mercapto Benzothiazole 155-04-4	Benzothiazole 2-(4-morpho linyldithio)- 95-32-9	Benzothiazole Disulfide 120-78-5 (SIDS)
Hydrolysis	No data	0-15 % after 7D	No data	No data	No data	37% after 7 D
Biodegradation	0% after 28 D (100 mg/l) >65% after 21 D (0.8mg/l)	< 1 % after 28 D	No data	No data	No data	0.2 % after 28 D
Photodegradation	T ½ = 4.5D	T ½ = 3.2 hr (indirect) T ½ = 0.5 hr (direct)	T ½ = 3.2 hr	T ½ = 1.4 hr	T ½ = 0.37 hr (indirect)	T ½ = 0.4 hr
Fugacity Level III (distribution)						
Air	2.9 %	0.507 %	0.507 %	0.132 %	< 0.1 %	< 0.1 %
Water	40.2 %	35.9 %	35.9 %	19.1 %	36.6 %	17.2 %
Soil	56.8 %	63.4 %	63.4 %	55.9 %	63.3 %	72.7 %
Sediment	0.122 %	0.172 %	0.172 %	24.9 %	0.09 %	10.2%

= Non-sponsored chemicals used for data purposes only

Table 3. Matrix of Available and Adequate Data on Benzothiazole-based Thiazoles Category
Ecotoxicity

Endpoint	Benzothiazole **95-16-9**	2-Mercapto benzothiazole **149-30-4**	Sodium 2-mercapto Benzothiazole **2492-26-4**	Zinc mercapto Benzothiazole **155-04-4**	Benzothiazole 2-(4-morpho linyldithio)- **95-32-9**	Benzothiazole Disulfide **120-78-5**
Acute Fish Toxicity (96 hr LC50)	*P. promelas* 64 mg/l *B. rerio* 65.5-66 mg/l	*P. promelas* 11 mg/l *B. rerio* 0.8 – 3.2 mg/l	*L. macrochirus* 12-15 mg/l *O. mykiss* 2.58-3.16 mg/l	*L. idus* 10-50 mg/l (48 hr)	Fish 512 mg/l (ECOSAR)	*P. promelas* > 1000 mg/l *O. mykiss* 66 mg/l
Acute Invertebrate Toxicity (48 hr LC50)	No data	*Daphnia* 2.9 - 4.1 mg/l	*Daphnia* 19 mg/l	*Daphnia* 0.54 mg/l (ECOSAR)	*Daphnia* 533 mg/l (ECOSAR)	*Daphnia* > solubility
Algal Toxicity (96 hr EC50)	No data	*S. capricornutum.* 0.25 mg/l	*S. capricornutum.* 0.3 mg/l	Green Algae 0.420 mg/l (ECOSAR)	Green Algae 325.5 mg/l (ECOSAR)	*S. subspicatus* > solubility

= Non-sponsored chemicals used for data purposes only

ECOSAR = Modeling Program - version 0.99e. Meylan W. and Howard P. (1999) Syracuse Research Corporation. Environmental Science Center, 6225 Running Ridge Road, North Syracuse, NY 13212-2510.

Table 4. Matrix of Available and Adequate Data on Benzothiazole-based Thiazoles Category
Mammalian Toxicity

Endpoint	Benzothiazole **95-16-9**	2-Mercapto benzothiazole **149-30-4**	Sodium 2-mercapto benzothiazole **2492-26-4**	Zinc mercapto Benzothiazole **155-04-4**	Benzothiazole 2-(4-morpho linyldithio)- **95-32-9**	Benzothiazole Disulfide **120-78-5**
Acute Toxicity						
Oral LD50	177-479 mg/kg bw (rat)	2830 – 3800 mg/kg bw (rat)	5200 mg/kg (rat) (45-50% substance content)	> 10000 mg/kg bw (rat)	No data	> 7940 mg/kg bw (rat)
Dermal LD50	933– 1233 mg/kg bw (rat)	> 7940 mg/kg bw (rabbit)	> 5010 mg/kg bw (rabbit) (45-50% substance content)	> 7940 mg/kg bw (rabbit)	No data	> 7940 mg/kg bw (rabbit)
Inhalation LC50	ca. 5 mg/l (4 hrs) (rat)	> 1.27 mg/l (4 hrs) (rat)	> 8.2 mg/l (6 hrs) (rat) (22% substance content)	No data	No data	No data
Mutagenicity – gene mutation	Ames = negative	Ames = negative Yeast = negative *E. coli* = negative	Ames = negative Balb3T3 = negative Yeast = negative	Ames = negative Yeast = negative	Ames = negative Balb3T3 = negative	Ames = negative *E. coli* = negative
Mutagenicity – chromosome aberration	No data	MLA = negative Dominant Lethal = negative MNT = negative	No data	No data	No data	MLA = negative
Repeated Dose	No data	90 D NOAEL = 375 mg/kg bw (rat) 28 D NOAEL = 714 mg/kg (rat)	No data	No data	No data	17 month NOAEL = 237 – 464 mg/kg bw (mouse) 90 D NOAEL – 100 mg/kg bw (rat)
Reproductive Toxicity	No data	NOAEL P, F1,F2= < 179 mg/kg bw Repro NOEC = 1071 mg/kg bw (rat)	No data	No data	No data	LOAEL = 200 mg/kg bw (rat)
Developmental Toxicity	No data	NOAEL = 1800 – 2200 mg/kg bw (rat)	No data	No data	No data	NOEL = 596 mg/kg bw (rat)

= Non-sponsored chemicals used for data purposes only

Table 5. Test Plan for the Benzothiazole-based Thiazoles Category

Endpoint	Benzothiazole 95-16-9	2-Mercapto benzothiazole 149-30-4	Sodium 2-mercapto Benzothiazole 2492-26-4	Zinc mercapto Benzothiazole 155-04-4	Benzothiazole 2-(4-morpho linyldithio)- 95-32-9	Benzothiazole Disulfide 120-78-5
Environmental Fate						
Hydrolysis	N	A	C	C	C	A
Bio-degradation	A	A	C	C	C	A
Photo-degradation	A	A	A	A	A	A
Fugacity	A	A	A	A	A	A
Ecotoxicology						
Acute Fish Toxicity	A	A	A	A	S	A
Acute Invertebrate	N	A	A	S	S	A
Alga Toxicity	N	A	A	S	S	A
Mammalian Toxicology						
Acute Toxicity	A	A	A	A	C	A
Mutagenicity : gene mutation	A	A	A	A	A	A
Mutagenicity: chromosome	N	A	C	C	C	A
Repeated Dose	N	A	C	C	C	A
Reproductive Toxicity	N	A	C	C	C	A
Developmental Toxicity	N	A	C	C	C	A

= Non-sponsored chemicals used for data purposes only

Key for symbols in table:
A = Adequate data available
C = Use of Category Approach
T = Testing to be done
S = Structure activity relationship
N = No testing; SIDS chemical

Background Information: Manufacturing and Commercial Applications

Manufacturing

The Benzothiazole-based Thiazoles are all made in batch processes using Carbon Disulfide, Aniline and Sulfur as starting materials. That reaction produces Crude MBT (90%) and BTH (5%). Crude MBT is treated with aqueous Sodium Hydroxide to produce NaMBT. The NaMBT solution is reacted with Zinc Sulfate to produce ZMBT, Sulfuric Acid to produce purified MBT, and Chlorine to produce MBTS. MBTS is reacted with Morpholine and additional Sulfur to produce MORFAX.

Commercial Applications

Benzothiazole-based Thiazole rubber chemicals have been manufactured in the United States since the late 1920s, and are widely used throughout the industry due to their excellent stability, functionality and low cost. Over 90% of all usage is as cure-rate accelerators in the manufacture of tires (sidewall, tread and retread, carcass, belt skim, liner, bead filler/chafer, and base tread) and industrial rubber products (automotive extruded sponge, latex and foam, insulated wire, insulation jackets, molded and mechanical goods). Latex applications include shoe soles, elastic, carpet backing, gloves and tubing. The typical usage for a cure-rate accelerator application ranges from 0.5 to 5 parts accelerator per 100 parts of rubber (phr). The Specialty Chemical (non-rubber) applications include chemical intermediates for rubber additives, herbicides and pharmaceuticals, as industrial water treatment additives, for ore chelation/flotation/separation, lubrication additives, as a corrosion inhibitor in ethylene glycol-based automotive antifreeze and as topical veterinary drugs.

Compounds in this category are sold only to large industrial users as ingredients or reagents for their products or processes. There are no direct consumer applications for this class of compounds, and therefore no direct sales to the general public.

The following chemicals have been “Regulated for Use” by the Food and Drug Administration in various food-contact applications:

175.105	Components of Adhesives	MBT, ZMBT, MBTS, NaMBT
176.200	Defoaming Agents, Coatings	NaMBT
176.210	Defoaming Agents, Paper	NaMBT
176.300	Slimicides	MBT
177.2600	Rubber Articles	MBT, ZMBT, MBTS
178.3120	Animal Glue	ZMBT, NaMBT

Shipping/Distribution

Benzothiazole-based thiazole compounds are shipped extensively throughout the world from manufacturing plants located in the United States, South America, Eastern and Western Europe, Japan and China.

Worker/Consumer Exposure

The rubber and plastics additives industry has a long safety record and only sophisticated industrial users handle these materials. Exposure of workers handling Benzothiazole-based thiazole materials is likely to be the highest in the area of material packaging rather than from chemical manufacturing. These materials are made as pastilles (pellets), powders, flakes, solids and liquids. Product forms that minimize dust generation, coupled with the mechanized materials handling systems of the large industrial users, combine to keep exposures to minimum levels. However, during material packout at the manufacturing site and, to a somewhat lesser degree during weigh-up activities at the customer site, there is a potential for skin and inhalation exposure (nuisance dust is the primary route of worker exposure) and also dermal contact with liquid forms.

Consumer exposure is minimal. Only very small amounts are used in rubber processing, and the materials themselves become bound in the rubber matrix during the vulcanization process. The most likely route of consumer exposure is skin contact from rubber or latex articles. Skin irritation, or possibly an allergic skin reaction may occur, but only in sensitive individuals subjected to prolonged and repeated exposure, especially under moist conditions. In the specialty application of ethylene glycol-based automotive antifreeze, the amount used is less than 3%.

AR201-13324B

I U C L I D

D a t a S e t

Existing Chemical	ID: 149-30-4
CAS No.	149-30-4
EINECS Name	benzothiazole-2-thiol
EINECS No.	205-736-8
TSCA Name	2(3H)-Benzothiazolethione
Molecular Formula	C7H5NS2

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

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

Memo: Rubber and Plastics Additives (RAPA) HPV Panel

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

Number of Pages: 62

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: American Chemistry Council (formerly Chemical Manufacturers Association) Rubber and Plastic Additives (RAPA) HPV Panel
Street: 1300 Wilson Boulevard
Town: 22209 Arlington, VA
Country: United States
Phone: 703-741-5600
Telefax: 703-741-6091

05-OCT-2001

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

05-OCT-2001

Type: cooperating company
Name: Ciba Specialty Chemicals Corporation
Country: United States

05-OCT-2001

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

05-OCT-2001

Type: cooperating company
Name: Flexsys America L.P.
Country: United States

05-OCT-2001

Type: cooperating company
Name: Noveon, Inc (formerly BF Goodrich)
Country: United States

05-OCT-2001

Type: cooperating company
Name: R.T. Vanderbilt Company, Inc.
Country: United States

05-OCT-2001

Type: cooperating company
Name: The Goodyear Tire & Rubber Company
Country: United States

05-OCT-2001

Type: cooperating company
Name: The Lubrizol Corporation
Country: United States

05-OCT-2001

Type: cooperating company
Name: UOP, LLC.
Country: United States

05-OCT-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: >= 95 % w/w
05-OCT-2001

1.1.0 Details on Template
-

1.1.1 Spectra
-

1.2 Synonyms

2(3H)-benzothiazolethione
20-OCT-1999

2-mercaptobenzothiazole
20-OCT-1999

MBT
20-OCT-1999

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

Value: = 180.2 - 181.7 degree C
Decomposition: no
Method: other: Handbook value
GLP: no data
Testsubstance: other TS: 2-Mercaptobenzothiazole; purity not noted
Reliability: (2) valid with restrictions
Data from Handbook or collection of data
Flag: Critical study for SIDS endpoint
05-OCT-2001 (2)

Value: ca. 180 degree C
Decomposition: no
Sublimation: no
Method: other
GLP: no data
Source: Bayer AG Leverkusen
19-MAY-1994 (3)

2.2 Boiling Point

Value: > 260 degree C at 1013 hPa
Decomposition: yes
GLP: no data
Remark: Decomposes above 260 degrees centigrade.
Source: Bayer AG Leverkusen
Flag: Critical study for SIDS endpoint
19-MAY-1994 (3)

2.3 Density

Type: density
Value: = 1.42 g/cm3 at 20 degree C
Method: other: Handbook value
GLP: no data
Testsubstance: other TS: 2-Mercaptobenzothiazole; purity not noted
Reliability: (2) valid with restrictions
Data from Handbook or collection of data
Flag: Critical study for SIDS endpoint
05-OCT-2001 (1) (4)

Type: density
Value: = 1.42 - 1.5 g/cm3 at 25 degree C
GLP: no data
Source: Bayer AG Leverkusen
19-MAY-1994 (3)

2.3.1 Granulometry
-

2.4 Vapour Pressure

Value: < .000003 hPa at 25 degree C
Method: OECD Guide-line 104 "Vapour Pressure Curve"
Year: 1981
GLP: yes
Testsubstance: other TS: 2-Mercaptobenzothiazole; purity not noted
Remark: Method similar to OECD test method 104. This procedure employed the gas saturation technique.
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
05-OCT-2001 (5)

2.5 Partition Coefficient

log Pow: 2.862 at 25 degree C
Method: other (calculated): KOWWIN Program (v1.65)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
05-OCT-2001 (6)

log Pow: = 2.34 - 2.5
Method: other (measured)
Year: 1980
GLP: yes
Testsubstance: other TS: 2-Mercaptobenzothiazole; purity not noted
Source: Bayer AG Leverkusen
Test condition: Method did not follow OECD guidelines. Samples analyzed at one test concentration only.
Reliability: (2) valid with restrictions
Guideline study with acceptable restrictions
Flag: Critical study for SIDS endpoint
05-OCT-2001 (7)

log Pow: 2.41
Method: other (measured)
Year:
GLP: no data
26-APR-2001 (8)

2.6.1 Water Solubility

Value: = 118 mg/l at 25 degree C
pH: = 7
Method: other
Year: 1980
GLP: yes
Testsubstance: other TS: purity not noted
Remark: Water solubility measured at 3 pHs; 51 ppm at pH 5, 118 ppm at pH 7 and 900 ppm at pH 9.
Source: Bayer AG Leverkusen
Reliability: (2) valid with restrictions
Comparable to Guideline study
Flag: Critical study for SIDS endpoint
05-OCT-2001 (7)

Value: = 150 mg/l
Method: other
GLP: no data
Source: Bayer AG Leverkusen
19-MAY-1994 (9)

2.6.2 Surface Tension
-

2.7 Flash Point

Value: ca. 252 degree C
Type: open cup
Method: other
Year:
GLP: no data
Source: Bayer AG Leverkusen
19-MAY-1994 (3)

2.8 Auto Flammability
-

2.9 Flammability
-

2.10 Explosive Properties
-

2.11 Oxidizing Properties
-

2.12 Additional Remarks
-

3.1.1 Photodegradation

Type: water
Light source: Sun light
Conc. of subst.: .495 mg/l at 36 degree C
DIRECT PHOTOLYSIS
Halflife t1/2: 31.1 minute(s)
Degradation: 86 % after 90 minute(s)
INDIRECT PHOTOLYSIS
Sensitizer: water with additives
Degradation: = 91 % after 90 minute(s)
Method: EPA OTS 795.7000
Year: 1989 GLP: yes
Test substance: other TS: 2-mercaptobenzothizole; purity = 98.2%
Method: Federal register 53(173) page 34522-34530.
Test condition: Indirect photolysis measurement was with added humic acid. Half-life estimated to be 27.4 minutes.
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
05-OCT-2001 (10)

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1560000 molecule/cm3
Rate constant: .0000000000406348 cm3/(molecule * sec)
Degradation: 50 % after 3.2 hour(s)
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-OCT-2001 (6)

Type: other: dilute phosphate buffer
Light source: Sun light
Conc. of subst.: 11.1 mg/l at 20 degree C
DIRECT PHOTOLYSIS
Halflife t1/2: .1 - .2 day
Degradation: 100 % after
Quantum yield: 0
INDIRECT PHOTOLYSIS
Sensitizer: other: dissolved organic matter
Conc. of sens.: 10 mg/l
Rate constant: ca. 3.1 cm3/(molecule * sec)
Degradation: 98 % after
Method: other (measured): test conditions undocumented
Year: 1992 GLP: no data
Test substance: no data
Remark: for direct-ph 7, rate constant 8.1-8.7; for indirect-initial conc.=1.9 mg/l, temp=1-10C, total solar radiation=36.3E/m2, pH=7, t 1/2=.28-.44 day, quantum yield=.0013; similar results obtained when natural water was used -quantum

yield=.0015 and 100% reduction; products formed with and without sensitizer and in natural water- benzothiazole (28-47%), 2-hydroybenzothiazole (4-5%) and unidentified product
Source: Bayer AG Leverkusen
18-JAN-1995 (11)

Type: other: ethanol
Light source: other: Hanovia mercury lamp-UV irradiation
Conc. of subst.: 860 mg/l
Method: other (measured): Parkanyi, C. et al protocol; see test conditions
Year: 1985 GLP: no data
Test substance: no data
Remark: Final product was benzothiazole sulfate with solutions of methanol, ethanol or acetonitrile; When dry benzene or toluene was the reaction medium bis-(2-benzothiazolyl) disulfide was formed that could then be degraded to benzothiazole; oxygen is necessary for this reaction to take place and water is needed for last step
Source: Bayer AG Leverkusen
Test condition: immersion-well type; water cooled Ace Glass photochemical reactor; air saturated 96% ethanol; irradiated 22 hours; 450 watts
03-MAR-1994 (12)

Type: other: filter paper
Light source: other: germicidal lamp
Method: other (measured): Mitchell, E.C. protocol; see test conditions
Year: 1961 GLP: no data
Test substance: no data
Remark: classified as "little or no degradation"
Source: Bayer AG Leverkusen
Test condition: 10 mg quantities of a pesticide chemical are spotted on filter paper and the spot is exposed to a germicidal light (30 watt)
03-MAR-1994 (13)

Type: water
Light source: Sun light
Conc. of subst.: 1.1 mg/l
DIRECT PHOTOLYSIS
Halflife t1/2: 3.7 hour(s)
Method: other (measured): test conditions undocumented
Year: 1980 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: Four photodegradation by-products were observed.
Source: Bayer AG Leverkusen
18-JAN-1995 (14)

3.1.2 Stability in Water

Type: abiotic
Degradation: 15 % after 7 day
at pH 7
Method: other: Monsanto protocol
Year: 1985 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Source: Bayer AG Leverkusen
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
05-OCT-2001 (15)

Type: abiotic
Degradation: 0 % after 7 day
Method: other: according to Analytic Bio-Chemistry Labs Protocol
Year: 1984 GLP: no data
Test substance: other TS: 2-mercaptobenzothiazole, purity = 98%
Remark: No measurable hydrolysis after 7 days
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
05-OCT-2001 (16)

Type: biotic
Method: other: test conditions undocumented
Year: 1992 GLP: no data
Test substance: no data
Remark: 6 mg chemical; sediment 1.33 g dry weight/l H2O; Converted in low yield to 2-(methylthiobenzothiazole)
Source: Bayer AG Leverkusen
03-MAR-1994 (11)

3.1.3 Stability in Soil
-

3.2 Monitoring Data (Environment)

Type of measurement: other: monitoring paper mill
Medium: other: effluent
Method:
Concentration
Remark: 4 samples taken at various stages of treatment; conc. ranged from .025-.035 mg/l
Source: Bayer AG Leverkusen
03-MAR-1994 (17)

3.3.1 Transport between Environmental Compartments

Type: adsorption
Media: water - soil
Air (Level I):
Water (Level I):
Soil (Level I):
Biota (L.II/III):
Soil (L.II/III):
Method: other: Springborn Laboratories protocol; see test conditions
Year: 1989
Result: Results:

	Kd	Koc	Slope (1/n)	%Organic Matter
California Sandy Loam	4.38	677	0.855	1.1
California Clay Loam	5.73	326	0.808	3.0
California Sand	0.799	1360	1.137	0.1
Carver Sandy Loam	18.8	2130	0.594	1.5
Dartmouth Sand	23.0	3560	0.861	1.1
Weweantic Sand	18.3	2590	0.763	1.2

Kd = adsorprtion coefficient
Koc = adsorprtion coefficient based on organic carbon content
Test condition: Protocol followed US TSCA Test Standard 40 CFR Chapter 1, paragraph 796.2750.
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
05-OCT-2001 (18)

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	0.507	6.32	1000	7.72e-012
Water	35.9	360	1000	4.06e-013
Soil	63.4	360	1000	2.76e-012
Sediment	0.172	1.44e+003	0	2.71e-013

Persistence Time: 347 hr
Reaction Time: 405 hr
Advection Time: 2.44e+003 hr
Percent Reacted: 85.8
Percent Advected: 14.2
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint

05-OCT-2001 (6)

Type: adsorption
Media: water - soil
Air (Level I):
Water (Level I):
Soil (Level I):
Biota (L.II/III):
Soil (L.II/III):
Method:
Year:
Method: Aqueous solutions of MBT, initial concentrations ranging from 0.1 to 1.0 ppm, were equilibrated for 24 hours with four soils. K (adsorption coefficient) was calculated using the following equation
K= equilibrium concentration in soil / equilibrium concentration in water

The concentration in the water was measured using analytical method ES-80-M-15. The concentration in the soil was calculated by the difference.

Result:

Soil	K	95% confidence limits
Drummer silty clay loam	18	13-23
Spinks sandy loam	12	8-19
Ray silt loam	10	6-16
Lintonia sandy loam	7.5	5-11
Mean =	12	

Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
05-OCT-2001 (19)

3.3.2 Distribution
-

3.4 Mode of Degradation in Actual Use
-

3.5 Biodegradation

Type: aerobic
Inoculum: activated sludge, adapted
Concentration: 23.8 mg/l related to Test substance
Degradation: < 1 % after 28 day
Result: under test conditions no biodegradation observed
Method: EPA OTS 796.3100
Year: 1989 GLP: yes
Test substance: other TS: 2-mercaptobenzothiazole, purity = 98%
Remark: Gledhill method listed in U.S. TSCA regulations 40 CFR Ch 1 subpart D paragraph 796.3100
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
05-OCT-2001 (20)

Type: aerobic
Inoculum: other: sludge samplings from different sewage plants, rivers, bays and a lake
Concentration: 100 mg/l related to Test substance
Degradation: 2.5 % after 14 day
Method: OECD Guide-line 301 C "Ready Biodegradability: Modified MITI Test (I)"
Year: 1981 GLP: no data
Test substance: no data
Remark: related to BOD; sludge conc.: 30 mg/l
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint
05-OCT-2001 (21)

Type: aerobic
Inoculum: activated sludge, adapted
Concentration: 18 mg/l related to Test substance
Degradation: 0 - 5 % after 35 day
Result: under test conditions no biodegradation observed
Method: other: CO2 evolution method listed in U.S. TSCA regulations 40 CFR Ch 1 subpart D paragraph 796.3100.
Year: GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Remark: Sample run in triplicate; 0%, 2%, and 5% theoretical carbon dioxide evolution obtained with an average of 2%.
Source: Bayer AG Leverkusen
18-JAN-1995 (22)

Type: aerobic
Inoculum: other: water and sediment from nearby creek, agricultural land and industrial site with sediment.
Concentration: 1 mg/l related to Test substance
Degradation: 81 % after 56 day
Result: other: Primary degradation was estimated to be 81% after 8 weeks.Sterile samples also degraded.
Method: other: SRI protocol; see test conditions
Year: 1985 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Bayer AG Leverkusen
Test condition: River die-away test.
18-JAN-1995 (23)

Type: aerobic
Inoculum: activated sludge
Concentration: 3 mg/l related to Test substance
Result: other: 3 mg/l inhibited oxidation of ammonia by 75%.
Method: other: see test conditions
Year: 1966 GLP: no data
Test substance: no data
Remark: The concentration of the oxidized form, benzothiazole disulphide, had to be about 10 times greater than that of MBT to give 75% inhibition of ammonia oxidation.
Source: Bayer AG Leverkusen
Test condition: 250 ml flasks at 25 degrees Celsius shaker for 2-4 hours.
18-JAN-1995 (24)

Type: aerobic
Inoculum: activated sludge
Concentration: 5 mg/l related to Test substance
Result: other: 74% inhibition of the nitrifying activity of activated sludge
Method: other: see test conditions
Year: 1966 GLP: no data
Test substance: no data
Remark: 5 mg/l MBT produced 74% inhibition, but in the presence of 5 mg/l zinc as zinc sulphate, which itself was not inhibitory, MBT was noninhibitory.
Source: Bayer AG Leverkusen
Test condition: 250 ml flasks at 25C in a shaker for 2-4 hours.
26-APR-1994 (24)

Type: aerobic
Inoculum: activated sludge
Concentration: 20 mg/l related to Test substance
Method: other: see test conditions
Year: 1966 GLP: no data
Test substance: no data
Source: Bayer AG Leverkusen
Test condition: Sewage containing MBT was supplied daily to a fill-and-draw plant. Initial period of 9 weeks MBT conc 2 mg/L, was increased to 20 mg/L for 7 weeks. Results suggest that during experiment, a strain of Nitrosomonas developed which was far less susceptible to MBT than that in the control sludge. Whereas 2 mg/L MBT inhibited control sludge by 75%, over 40 mg/L was necessary to produce the same effect on sludge which was previously exposed to 20 mg/L MBT. There was no evidence MBT was being decomposed in the sewage.
03-MAR-1994 (24)

Type: aerobic
Inoculum: other: soil
Concentration: 1 g/l related to Test substance
Result: other: completely retarded microbial growth of soil microbes at 0.1%
Method: other: see test conditions
Year: 1984 GLP: no data
Test substance: no data
Remark: After three months, MBT completely retarded microbial growth of soil microbes at 0.1%. Toxicity level for MBT in agar: 4-day LD50 & 14-day LD50 < = 0.1%.
Source: Bayer AG Leverkusen
Test condition: Three techniques used for exposing rubber additives to John Innes No. 1 Soil. 1st involved placing powdered additives onto non-biodegradable polycarbonate membranes w/a 12 um pore diameter & placing membranes onto the soil w/powders on the upper surface. 2nd involved embedding powdered additives onto a thin layer (0.3 cm) of epoxy resin poured onto aluminum foil. During the curing process, excess of powder was poured onto resin. When cured, excess powder was shaken off resin which was cut and placed with the additive in contact with the soil. 3rd technique involved incorporating additives into an agar medium & inoculating medium with soil extract.
26-APR-1994 (25)

Type: aerobic
Inoculum:
Concentration: 20 mg/l related to Test substance
Degradation: 0 - 12 % after 3 day
Method: other: see test conditions
Year: GLP: no data
Test substance: no data
Remark: 2-MBT was tested for degradability in river water by 4 different institutes. The results were 0%, 3%, 11% & 12%. It was also tested in sea water with the following results: 0%, 21%, 41%, 10%.
Partial translation (abstract and results table) of a Japanese article.
Source: Bayer AG Leverkusen
Test condition: Method was listed as the "cultivation method".
18-JAN-1995 (26)

Type: aerobic
Inoculum:
Result: other: listed as resistant substance in U.K.
Method: other: test conditions undocumented
Year: 1975 GLP: no data
Test substance: no data
Source: Bayer AG Leverkusen
03-MAR-1994 (27)

Type:
Inoculum:
Result: other: listed as degradation resistant
Method: other: MITI
Year: GLP: no data
Test substance: no data
Source: Bayer AG Leverkusen
26-APR-1994 (28)

3.6 BOD5, COD or BOD5/COD Ratio
-

3.7 Bioaccumulation

Species: Cyprinus carpio (Fish, fresh water)
Exposure period: 42 day
Concentration: .1 mg/l
BCF: < .8
Elimination: no data
Method: OECD Guide-line 305 C "Bioaccumulation: Test for the Degree of Bioconcentration in Fish"
Year: 1981 GLP: no data
Test substance: no data
Remark: when test conc. .01 mg/l BCF < 8.0
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
Guideline study
05-OCT-2001 (21)

Species: Cyprinus carpio (Fish, fresh water)
Exposure period: at 15 degree C
Concentration: .56 mg/l
BCF:
Elimination: yes
Method: other: Hashimoto, K. et al protocol; see test conditions
Year: 1978 GLP: no data
Test substance: other TS: 14C; 98.5% pure
Remark: about 20% excreted at 1h, 35% at 2h, 75% at 24h and 77% at 72h; fish that were fed had 100% excretion at 72hr; chemical oxidized to C-2,2,dithiobis[benzothiazole]
Source: Bayer AG Leverkusen
Test condition: fish starved 2 days prior to test; 30L water; water renewed at periodic intervals, some fish fed after administration of chemical, chemical administered with a catheter into intestine
18-JAN-1995 (29)

Species: Cyprinus carpio (Fish, fresh water)
Exposure period: 56 day at 25 degree C
Concentration:
BCF:
Elimination: no data
Method: other: test conditions undocumented
Year: 1978 GLP: no data
Test substance: no data
Remark: "confirmed to be non accumulative or low accumulative" ie. BCF did not increase a few hundred times during the 56 day exposure
Source: Bayer AG Leverkusen
Test condition: length 10 cm; weight 30 g; DO 7 mg/l
18-JAN-1995 (30)

3.8 Additional Remarks
-

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: static
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
NOEC: 4.2
LC50: 11
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1984 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: all conc. tested were above solubility
C.I. 8.3-15 mg/l; 24h-LC50: 18 mg/l; 48h-LC50: 13mg/l
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
05-OCT-2001 (31)

Type: static
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: yes
LC0: .8
LC100: 3.2
Method: other: UBA-Verfahrensvorschlag "Lethale Wirkung beim ZebrabaerblingBrachydanio rerio (LC0, LC50< LC100, 48-96 h), Mai 1984
Year: 1984 GLP: no data
Test substance: other TS: 2-Mercaptobenzothiazole; purity not noted
Remark: geometric mean: 1.6 mg/l
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
05-OCT-2001 (32)

Type: static
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: .75
Method: other: Bionomics Laboratory protocol; see test conditions
Year: 1976 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Remark: C.I. 0.55-1 mg/l; 24h-LC50: 0.92 mg/l; 48h-LC50: 0.75 mg/l
Source: Bayer AG Leverkusen
Test condition: carrier-acetone; 15L water; 10 fish/vessel; length 3.7 cm; no food; no aeration; temp 12 degrees Celsius
05-OCT-2001 (33)

Type: static
Species: Lepomis macrochirus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: 1.5
Method: other: Bionomics Laboratroy protocol; see test conditions
Year: 1976 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Remark: C.I. 1.2-1.9 mg/l; 24h-LC50: 3.4 mg/l; 48h-LC50: 2.1 mg/l
Source: Bayer AG Leverkusen
Test condition: carrier-acetone; 15L water; 10 fish/vessel; length 3.8 cm; no food; no aeration; temp 22 degrees Celsius
05-OCT-2001 (33)

Type: semistatic
Species: Cyprinus auratus
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no data
LC50: 2
Method: other: test conditions undocumented
Year: 1983 GLP: no data
Test substance: no data
Source: Bayer AG Leverkusen
05-OCT-2001 (34)

Type: flow through
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period: 8 day
Unit: mg/l Analytical monitoring: yes
LC50: .67
Method: other: Springborn Laboratory protocol; see test conditions
Year: 1981 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Remark: C.I. 0.54-0.83 mg/l; 24h-LC50: 1.14 mg/l; 48h-LC50: 0.73 mg/l
Source: Bayer AG Leverkusen
Test condition: continuous flow; 19L aquaria; 10 fish/conc; fed brine shrimp daily
05-OCT-2001 (35)

4.2 Acute Toxicity to Aquatic Invertebrates

Type:	
Species:	Daphnia magna (Crustacea)
Exposure period:	48 hour(s)
Unit:	mg/l Analytical monitoring: no
NOEC:	1.8
EC50:	4.1
Method:	OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year:	1984 GLP: yes
Test substance:	as prescribed by 1.1 - 1.4
Remark:	C.I. for EC50: 3.6-4.7 mg/l; 24h-LC50: 7.0 mg/l
Source:	Bayer AG Leverkusen
Reliability:	(1) valid without restriction GLP guideline study
Flag:	Critical study for SIDS endpoint

05-OCT-2001 (36)

Type:	
Species:	Daphnia magna (Crustacea)
Exposure period:	48 hour(s)
Unit:	mg/l Analytical monitoring: yes
NOEC:	1.9
EC50:	2.9
Method:	other: "Protocol for Conducting a Static Acute Toxicity Test with Daphnia magna Following FIFRA Guideline 72", SLI Protocol #010190/FIFRA 72-2 DM SA and protocol amendment #1 dated 9 January 1992
Year:	1992 GLP: yes
Test substance:	other TS: 100 % (2-Mercaptobenzothiazole (ROKON), Lot #N9H 211)
Remark:	24h-EC 50: 3.9 mg/l Analytical monitoring: HPLC
Source:	Bayer AG Leverkusen
Reliability:	(1) valid without restriction
Flag:	Critical study for SIDS endpoint

05-OCT-2001 (37)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species:	Selenastrum capricornutum (Algae)
Endpoint:	biomass
Exposure period:	96 hour(s)
Unit:	mg/l Analytical monitoring: no
EC50:	.25
Method:	OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year:	1984 GLP: no data
Test substance:	as prescribed by 1.1 - 1.4
Remark:	C.I. 0.06-0.98 mg/l; in vivo chlorophyll results - 24 and 48h-EC50 >0.3<0.6 mg/l, 96h-EC50: 0.23 mg/l
Source:	Bayer AG Leverkusen
Test condition:	temp 24 degrees Celsius; 4000 lux; Algal Assay Media; init. inoc. 10000 cells/ml; "cool" white lights
Reliability:	(1) valid without restriction Guideline study
Flag:	Critical study for SIDS endpoint

05-OCT-2001 (38)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type:	aquatic
Species:	Tetrahymena sp. (Protozoa)
Exposure period:	24 hour(s)
Unit:	mg/l Analytical monitoring: no
EC50:	10
Method:	other: Yoshioka, Y. protocol; see test conditions
Year:	1985 GLP: no data
Test substance:	no data
Source:	Bayer AG Leverkusen
Test condition:	temp. 30 degrees Celsius; sterile medium of 2% protose peptone; 60 µmol/l; no agitation; count cell numbers; conc. ratio of 1.8 in 10 ml media

18-JAN-1995 (39)

Type:	other: undefined and synthetic media
Species:	other bacteria: several genera
Exposure period:	
Unit:	Analytical monitoring: no data
Method:	other: test conditions undocumented
Year:	1976 GLP: no data
Test substance:	no data
Remark:	complete inhibition at 50-1000 µg/ml; partial inhibition from 25-1000 µg/ml
Source:	Bayer AG Leverkusen

18-JAN-1995 (40)

Type: other: unknown
Species: Aspergillus niger (Fungi)
Exposure period:
Unit: Analytical monitoring: no data
Method: other: test conditions undocumented
Year: 1975 GLP: no data
Test substance: no data
Remark: Inhibits sporulation; also inhibits several other bacteria
Source: Bayer AG Leverkusen
04-MAY-1994 (41)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

Species: Oncorhynchus sp.
Endpoint: other: embryo survival,viability, length
Exposure period: 89 day
Unit: mg/l Analytical monitoring: yes
MATC : .041 - .078
Method: other: Federal Register 50:797.1600
Year: 1989 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: max. accept. tox. concentration for larval length; no effect on embryo viability or survival.
Test condition: test lasted 60 days post hatch; 24-80 foot candles; temp. 12 degrees Celsius
Reliability: (1) valid without restriction
27-APR-2001 (42)

4.5.2 Chronic Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)
Endpoint: reproduction rate
Exposure period: 21 day
Unit: mg/l Analytical monitoring: yes
NOEC: .34
EC50: > .47
Method: OECD Guide-line 202, part 2 "Daphnia sp., Reproduction Test"
Year: 1989 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: Maximum accept. conc.>0.25<0.47 mg/l; geometric mean: 0.34 mg active ingredient/liter
Test condition: carrier acetone; 50% dilutions; 1.8L vessels; 30-70 foot candles; 16 hours light; temp. 20 degrees Celsius
Reliability: (1) valid without restriction
27-APR-2001 (43)

Species: Daphnia magna (Crustacea)
Endpoint: reproduction rate
Exposure period: 21 day
Unit: mg/l Analytical monitoring: no
NOEC: ca. .22
EC50: ca. 2.22
Method: OECD Guide-line 202, part 2 "Daphnia sp., Reproduction Test"
Year: 1987 GLP: no
Test substance: other TS: 99.45 %
Source: Bayer AG Leverkusen
Test condition: concentrations tested: 0.07, 0.22, 0.7, 2.22, and 7 mg/l. Preparation of stock solution: 100 mg of test substance were weighed into 1 l of water and dissolved over night by means of a magnetic stirrer.

18-JAN-1995 (32)

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:	
Sex:	
Number of Animals:	
Vehicle:	
Value:	= 3800 mg/kg bw
Method:	other
Year:	1975 GLP: no data
Test substance:	as prescribed by 1.1 - 1.4
Source:	Bayer AG Leverkusen
Flag:	Critical study for SIDS endpoint

05-OCT-2001 (44)

Type:	LD50
Species:	rat
Strain:	
Sex:	
Number of Animals:	
Vehicle:	
Value:	= 2830 mg/kg bw
Method:	other
Year:	1973 GLP: no data
Test substance:	as prescribed by 1.1 - 1.4
Source:	Bayer AG Leverkusen
Flag:	Critical study for SIDS endpoint

05-OCT-2001 (45)

Type:	LD50
Species:	mouse
Strain:	
Sex:	male
Number of Animals:	
Vehicle:	other: 0.5% carboxymethyl cellulose in normal saline
Value:	2000 mg/kg bw
Method:	
Year:	GLP:
Test substance:	other TS: ROTAX (purified MBT)
Method:	Mice were observed for 72 hours after a single oral exposure. LD50 values were calculated by the Cornfield and Mantel modification (1950) of the Karber method.
Flag:	Critical study for SIDS endpoint

05-OCT-2001 (46)

Type: LD50
Species: rat
Strain:
Sex: no data
Number of Animals:
Vehicle: no data
Value: > 500 mg/kg bw
Method:
Year: GLP:
Test substance: other TS: 2-mercaptobenzothiazole (purity not noted)
03-NOV-2000 (47)

Type: LDLo
Species: rabbit
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 7500 - 8750 mg/kg bw
Method: other
Year: 1955 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Bayer AG Leverkusen
23-FEB-1994 (48)

5.1.2 Acute Inhalation Toxicity

Type: LC50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Exposure time: 4 hour(s)
Value: > 1.27 mg/l
Method: other: Acute Inhalation Toxicity
Year: 1977 GLP: no data
Test substance: no data
Source: Bayer AG Leverkusen
Flag: Critical study for SIDS endpoint
05-OCT-2001 (49)

Type: LC50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Exposure time: 7 hour(s)
Value: > .722 mg/l
Method: other: Acute Inhalation Toxicity
Year: 1961 GLP: no data
Test substance: no data
Source: Bayer AG Leverkusen
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
05-OCT-2001 (50)

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rabbit
Strain:
Sex:
Number of Animals:
Vehicle:
Value: > 7940 mg/kg bw
Method: other
Year: 1975 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Bayer AG Leverkusen
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
05-OCT-2001 (44)

Type: LD50
Species: rabbit
Strain:
Sex:
Number of Animals:
Vehicle:
Value: > 7940 mg/kg bw
Method: other
Year: 1973 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Bayer AG Leverkusen
23-FEB-1994 (45)

5.1.4 Acute Toxicity, other Routes

Type:	LD50
Species:	mouse
Strain:	
Sex:	male
Number of Animals:	
Vehicle:	other: 0.5% carboxymethyl cellulose in normal saline
Route of admin.:	i.p.
Value:	437 mg/kg bw
Method:	
Year:	GLP:
Test substance:	other TS: ROTAX (purified MBT)
Method:	Mice were observed for 72 hours after a single i.p. injection. LD50 values were calculated by the Cornfield and Mantel modification (1950) of the Karber method.

03-NOV-2000 (46)

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:	other
Year:	1973 GLP: no data
Test substance:	as prescribed by 1.1 - 1.4
Source:	Bayer AG Leverkusen

06-SEP-1994 (45)

Species:	rabbit
Concentration:	
Exposure:	
Exposure Time:	
Number of Animals:	
PDII:	
Result:	not irritating
EC classificat.:	
Method:	other
Year:	1975 GLP: no data
Test substance:	as prescribed by 1.1 - 1.4
Source:	Bayer AG Leverkusen

06-SEP-1994 (44)

5.2.2 Eye Irritation

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: not irritating
EC classificat.:
Method: other
Year: 1975 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Bayer AG Leverkusen
06-SEP-1994 (44)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: not irritating
EC classificat.:
Method: other
Year: 1973 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Bayer AG Leverkusen
06-SEP-1994 (45)

5.3 Sensitization

Type: Buehler Test
Species: guinea pig
Number of Animals:
Vehicle:
Result: sensitizing
Classification:
Method: OECD Guide-line 406 "Skin Sensitization"
Year: 1992 GLP: no data
Test substance: other TS: 98 % purity
Source: Bayer AG Leverkusen
01-SEP-1994 (51)

Type: Buehler Test
Species: guinea pig
Number of Animals:
Vehicle:
Result: sensitizing
Classification:
Method: other
Year: 1988 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Bayer AG Leverkusen
06-SEP-1994 (52)

Type: Guinea pig maximization test
Species: guinea pig
Number of Animals:
Vehicle:
Result: sensitizing
Classification:
Method: OECD Guide-line 406 "Skin Sensitization"
Year: 1992 GLP: no data
Test substance: other TS: 98 % purity
Source: Bayer AG Leverkusen
01-SEP-1994 (51) (53) (54)

Type: Guinea pig maximization test
Species: guinea pig
Number of Animals:
Vehicle:
Result: sensitizing
Classification: sensitizing
Method: other
Year: 1970 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Bayer AG Leverkusen
23-FEB-1994 (55)

Type: Guinea pig maximization test
Species: guinea pig
Number of Animals:
Vehicle:
Result: sensitizing
Classification: sensitizing
Method: other
Year: 1968 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Bayer AG Leverkusen
23-FEB-1994 (56)

Type: Guinea pig maximization test
Species: guinea pig
Number of Animals:
Vehicle:
Result: sensitizing
Classification:
Method:
Year: 1992 GLP: no data
Test substance: no data
Source: Bayer AG Leverkusen
01-SEP-1994 (57)

Type: Guinea pig maximization test
Species: guinea pig
Number of Animals:
Vehicle:
Result: sensitizing
Classification:
Method:
Year: 1972 GLP: no data
Test substance: no data
Source: Bayer AG Leverkusen
06-SEP-1994 (58)

Type: Mouse local lymphnode assay
Species: mouse
Number of Animals:
Vehicle:
Result: sensitizing
Classification:
Method: other
Year: 1993 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Bayer AG Leverkusen
02-SEP-1994 (59)

Type: Mouse local lymphnode assay
Species: mouse
Number of Animals:
Vehicle:
Result: sensitizing
Classification:
Method: other: Skin Sensitization Test
Year: 1992 GLP: no data
Test substance: other TS: 98 % purity; dissolved in dimethyl formamide
Source: Bayer AG Leverkusen
01-SEP-1994 (51) (53) (54)

Type: Mouse local lymphnode assay
Species: mouse
Number of Animals:
Vehicle:
Result: sensitizing
Classification:
Method:
Year: 1989 GLP: no data
Test substance: other TS: dissolved either in DMSO or aqueous solvent
Source: Bayer AG Leverkusen
01-SEP-1994 (60)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result: not sensitizing
Classification: not sensitizing
Method: other
Year: 1976 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Bayer AG Leverkusen
23-FEB-1994 (61)

Type: other
Species: other
Number of Animals:
Vehicle:
Result:
Classification:
Method: other
Year: 1987 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: No T-cell response was noted in an in-vitro lymphocyte transformation assay.
Source: Bayer AG Leverkusen
02-JUN-1994 (62)

Type: other: occlusive epicutaneous test
Species: guinea pig
Number of Animals:
Vehicle:
Result: sensitizing
Classification:
Method: other: Skin Sensitization Test according to Brulos
Year: 1976 GLP: no data
Test substance: no data
Remark: Animals were applied 0.5 g test substance (in 1 % vaseline) to the interscapular region on alternate days for 4 weeks (10 applications, occlusive). At the first day of week 1 and 2, 0.1 ml Freund's adjuvans was injected intradermally. One

week after the last application animals were challenged with 0.5 g test compound epicutaneously (occlusive). The mean sensitizing index was 1.1 of 3.0 (maximal score). 50 % of animals were sensitized. Test substance was considered to be moderate sensitizing.

Source: Bayer AG Leverkusen

01-SEP-1994 (63)

5.4 Repeated Dose Toxicity

Species:	rat	Sex: male/female
Strain:	Fischer 344	
Route of admin.:	gavage	
Exposure period:	13 weeks	
Frequency of treatment:	5 days/week	
Post. obs. period:	3 days	
Doses:	188, 375, 750, 1500, or 3000 mg/kg bw	
Control Group:	yes	
NOAEL:	= 375 mg/kg bw	
LOAEL:	= 750 mg/kg bw	
Method:	other	
Year:		GLP: yes
Test substance:	other TS: mercaptobenzothizole, purity = 96.3%	

Remark: Because the hepatomegaly was not associated with histopathological findings, those dose levels with hepatomegaly but no other toxicity findings are considered to be no observable adverse effect levels (NOAELs) and are reported as NOELs.

Result: 1) 188 mg/kg bw/d: hepatomegaly, F.
2) 375 mg/kg bw/d: NOAEL; hepatomegaly, F.
3) 750 mg/kg bw/d: LOAEL; bw, decr, F; hepatomegaly, F.
4) 1500 mg/kg bw/d:
bw, decr;
hepatomegaly.

Source: Bayer AG Leverkusen

Reliability: (1) valid without restriction
GLP guideline study

Flag: Critical study for SIDS endpoint

05-OCT-2001 (64) (65)

Species: mouse Sex: male/female
Strain: B6C3F1
Route of admin.: gavage
Exposure period: 13 weeks
Frequency of treatment: 5 days/week
Post. obs. period: 3 days
Doses: 94, 188, 375, 750, or 1500 mg/kg bw
Control Group: yes
NOAEL: = 375 mg/kg bw
LOAEL: = 750 mg/kg bw
Method: other: well documented in Physiological research Laboratories 78-60-106002 (1981)
Year: GLP: yes
Test substance: other TS: mercaptobenzothizole, purity = 96.3%
Result: 1) 94 mg/kg bw/d:
no effects.
2) 188 mg/kg bw/d:
no effects.
3) 375 mg/kg bw/d:
NOEL;
no effects.
4) 750 mg/kg bw/d:
LOEL;
death, F.
5) 1500 mg/kg bw/d:
deaths.
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
05-OCT-2001 (64) (65)

Species: rat Sex: male/female
Strain: Sprague-Dawley
Route of admin.: oral feed
Exposure period: 4 weeks
Frequency of treatment: ad libitum
Post. obs. period:
Doses: 5000, 10000, 15000, 20000, or 25000 ppm
Control Group: yes
NOAEL: = 714 mg/kg bw
LOAEL: = 1071 mg/kg bw
Method: other
Year: 1988 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: 5000, 10000, 15000, 20000, 25000 ppm = 357, 714, 1071, 1429, 1786 mg/kg bw/d,
conversion factor is 14.
Result: 1) 5000 ppm:
NOEL;
no effect.
2) 10000 ppm:

NOEL;
no effects.
3) 15000 ppm:
LOEL;
bw gain, decr, M;
food consumption, decr, M.
4) 20000 ppm:
bw gain, decr;
food consumption, decr.
5) 25000 ppm:
bw gain, decr;
food consumption, decr.

Source: Bayer AG Leverkusen
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
05-OCT-2001 (66)

Species: rat Sex: male/female
Strain: Sprague-Dawley
Route of admin.: oral feed
Exposure period: 4 weeks
Frequency of treatment: continuous
Post. obs. period:
Doses: 4300, 9000, 14000, 19000, 25000 ppm
Control Group: yes, concurrent vehicle
LOAEL: 4300 ppm
Method: other
Year: GLP: no data
Test substance: other TS: 2-mercaptobenzothiazole (lot No. N8F-228)
Method: 2-mercaptobenzothiazole (lot No. N8F-228) was administered to Sprague-Dawley rats at target levels of 0, 5000, 10000, 15000, 20000, 25000 ppm in feed for 4 weeks. The test material was analysed neat and mixed with the diet. Averages for consumption were 425, 839, 1232, 1696, 2143 mg/kg (males) and 432, 874, 1320, 1703, 2058 mg/kg (females).

All animals were observed twice daily for mortality and moribundity. Detailed clinical observations and body weights were done weekly. All animals were given a thorough necropsy and livers were weighed.
Result: Observations included decreased weight gain and reduced food consumption, which were statistically significant in males at 15000 ppm and females at 20000 and 25000 ppm. Slightly heavier livers occurred in animals of both sexes at all levels.
05-OCT-2001 (67)

Species: mouse Sex: male/female
Strain: other: Slc: ddY
Route of admin.: oral feed
Exposure period: 20 months
Frequency of treatment: daily
Post. obs. period:
Doses: 30, 120, 480 or 1920 ppm (males: 3.6, 14.7, 57.9 or 289.4 mg/kg bw day; females: 3.6, 13.5, 58.9 or 248.0 mg/kg bw/day
Control Group: yes
NOAEL: = 120 ppm
Method: other: Repeated Dose Toxicity
Year: 1989 GLP: no data
Test substance: other TS: technical grade
Result: Inhibition of body weight gain was observed in the 1920 ppm-group of males from the initial stage of the treatment. No signigicant changes were seen between the controlnd athe treated groups in weights of organs and in several biochemical parameters of serum. Histopathologically, cell infiltration in the interstitium of kidney in the 1920 and 480 ppm-groups of the males was found at the 20th month.
Source: Bayer AG Leverkusen
05-OCT-2001 (68)

Species: mouse Sex: male
Strain: other: white
Route of admin.: i.p.
Exposure period: 1 week
Frequency of treatment: daily
Post. obs. period: none
Doses: 55 and 110 mg/kg
Control Group: yes, concurrent vehicle
NOAEL: 55 mg/kg bw
LOAEL: 110 mg/kg bw
Method: other
Year: GLP:
Test substance: other TS: ROTAX (purified MBT)
Method: Groups of male mice were dosed daily for one week by the i.p. route with oil suspensions of MBT. Control animals received daily injections of the same volume of cottonseed oil. At the end of one week, the animals were sacrificed, tissues were removed and examined histopathologically.
Result: There were no gross signs of toxicity at either dose level. All animals exhibited normal weight gain and behavior. Gross examination at necropsy revealed no significant injury to the vital organs. Microscopic examination of lungs, heart, thyroid and testes were normal. The kidney showed cloudy swelling and the livers revealed severe damage at the 110 mg/kg dose level.
05-OCT-2001 (46)

5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: Salmonella typhimuriumTA 97, TA98, TA100, TA102
Concentration: 1, 10, 100, 500, 1000, 5000 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year: 1983 GLP: yes
Test substance: other TS: MBT (purity not noted)
Result: There was no significant increase in revertant colonies and therefore no evidence for mutagenic activity in these assays. There was a toxic response to the test material at 5000 ug/plate and in most cases at 1000 ug/plate. The positive and negative controls were within acceptable limits.
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
05-OCT-2001 (69)

Type: Ames test
System of testing: TA98, TA100, TA1535, TA1537, TA1538
Concentration: up to 300 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: EPA OTS 798.5265
Year: 1986 GLP: yes
Test substance: other TS: MBT; lot #39-14B; purity not noted
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
05-OCT-2001 (70)

Type: Cytogenetic assay
System of testing: Chinese hamster ovary cells
Concentration: up to 500.5 ug/ml
Cytotoxic Conc.:
Metabolic activation: with and without
Result:
Method: other: Chromosome Aberration Test
Year: 1988 GLP: no data
Test substance: no data
Remark: result: negative (-S9 mix)
positive at > = 373,5 ug/ml (+ S9 mix)
Source: Bayer AG Leverkusen

Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint
05-OCT-2001 (64)

Type: Mouse lymphoma assay
System of testing: L5178Y mouse lymphoma cells
Concentration: up to 60ug/ml (with) and 70 ug/ml (without)
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: OECD Guide-line 476 "Genetic Toxicology: In vitro Mammalian Cell Gene Mutation Tests"
Year: 1984 GLP: no data
Test substance: other TS: 2-mercaptobenzothiazole (purity not stated)
Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint
05-OCT-2001 (71)

Type: Ames test
System of testing: TA98, TA100, TA1535, TA1537, TA1538
Concentration: up to 500 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: 1976 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Bayer AG Leverkusen
03-NOV-2000 (72)

Type: Escherichia coli reverse mutation assay
System of testing: Escherichia coli SD-4-73
Concentration: no data
Cytotoxic Conc.:
Metabolic activation: without
Result: negative
Method: other: Paper Disk Method
Year: 1958 GLP: no data
Test substance: no data
27-APR-2001 (73)

Type: Gene mutation in Saccharomyces cerevisiae
System of testing: D4 strain
Concentration: up to 500 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: 1976 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Bayer AG Leverkusen
23-FEB-1994 (72)

Type: HGPRT assay
System of testing: V79 Chinese hamster cells
Concentration: 50 - 300 ug/ml
Cytotoxic Conc.:
Metabolic activation: without
Result: negative
Method: other: 6-thioguanine Resistance Assay
Year: 1976 GLP: no data
Test substance: no data
Source: Bayer AG Leverkusen
01-SEP-1994 (74)

Type: HGPRT assay
System of testing: Chinese Hamster Ovary cells
Concentration: up to 333.33 ug/ml with S9 and up to 33.33 ug/ml without S9
Cytotoxic Conc.: with metabolic activation = 1000 ug/ml;
without metabolic activation = 333.33 ug/ml
Metabolic activation: with and without
Result: negative
Method: EPA OTS 798.5300
Year: 1986 GLP: yes
Test substance: other TS: MBT; lot #39-14B; purity not noted
Reliability: (1) valid without restriction
27-APR-2001 (75)

Type: Mouse lymphoma assay
System of testing: L5178Y
Concentration: up to 100 ug/ml
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: 1978 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Bayer AG Leverkusen
23-FEB-1994 (76)

Type: Mouse lymphoma assay
System of testing: L5178Y
Concentration: 3.75 - 150 ug/ml
Cytotoxic Conc.:
Metabolic activation: with and without
Result:
Method: other: TK Test
Year: 1985 GLP: yes
Test substance: other TS: solvent: DMSO
Remark: - S9: 1.8- to 8.7fold increases in the mutant frequency for treatments causing very high toxicity (less than 10 % relative growth).
+ S9: 1.7- to 2.7fold increases in the mutant frequency in the 7 - 20 % relative growth range; treatments with 150 ug/ml were lethal.
The results were evaluated as showing the test material to be weakly mutagenic at high toxicity.
Source: Bayer AG Leverkusen
06-SEP-1994 (77)

Type: Mouse lymphoma assay
System of testing: L5178Y
Concentration: up to 150 ug/ml
Cytotoxic Conc.:
Metabolic activation: with and without
Result:
Method: other: TK Test
Year: 1985 GLP: no data
Test substance: other TS: dissolved in ethanol
Remark: result: negative (- S9 mix)
positive at > = 5 ug/ml (+ S9 mix)
Source: Bayer AG Leverkusen
01-SEP-1994 (78)

Type: Mouse lymphoma assay
System of testing: L5178Y
Concentration: up to 150 ug/ml with S9 and up to 100 ug/ml without S9
Cytotoxic Conc.:
Metabolic activation: with and without
Result: ambiguous
Method: EPA OTS 798.5300
Year: 1986 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: Small increases in mutant frequency were observed but only at concentrations that also produced cytotoxicity.
Reliability: (1) valid without restriction
27-APR-2001 (79)

Type: Sister chromatid exchange assay
System of testing: Chinese hamster ovary cells
Concentration: up to 500.5 ug/ml
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: BrdUrd/dye technique
Year: 1988 GLP: no data
Test substance: no data
Source: Bayer AG Leverkusen
06-SEP-1994 (64)

5.6 Genetic Toxicity 'in Vivo'

Type: Dominant lethal assay
Species: rat Sex: male
Strain: CD-1
Route of admin.: oral feed
Exposure period: 13 weeks
Doses: 2500, 8750, or 15000 ppm
Result: negative
Method: EPA OPPTS 870.5450
Year: 1991 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Result: There were no findings that were indicative of dominant lethality.
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
05-OCT-2001 (80)

Type: Micronucleus assay
Species: mouse Sex: male/female
Strain: CD-1
Route of admin.: i.p.
Exposure period: single dose
Doses: 300 mg/kg bw
Result: negative
Method: EPA OTS 798.5395
Year: 1986 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Result: MBT was considered to not be clastogenic in this assay.
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
05-OCT-2001 (81)

Type: other: In vivo DNA binding study
Species: rat Sex: male/female
Strain: Fischer 344
Route of admin.: gavage
Exposure period: single dose
Doses: 375 mg/kg
Result: negative
Method: other
Year: GLP:
Test substance: other TS: radio-labelled 2-mercaptobenzothiazole (purity not noted)
Method: Male and female Fischer 344 rats were gavaged with 375 mg/kg MBT and sacrificed 8 hours later. DNA was extracted from the liver, adrenal glands, pituitary gland, pancreas, and bone marrow using standard exhaustive solvent extraction techniques. The amount of radioactivity associated with the DNA was determined.
Result: There was little or no binding of MBT with DNA in any of the tissues examined.
05-OCT-2001 (82)

Type: other: Drosophila mutagenicity assay
Species: Drosophila melanogaster Sex: no data
Strain: no data
Route of admin.: oral feed
Exposure period: 8 - 10 days
Doses: 20 - 40 mg/ml
Result:
Method: other: no data
Year: 1968 GLP: no data
Test substance: no data
Remark: The mutagenic activity included lethal, sublethal and visible mutations.
Result: mutation frequency: 2.5 +- 0.49 %;
no control group mentioned
Source: Bayer AG Leverkusen
05-OCT-2001 (83)

5.7 Carcinogenicity

Species: rat Sex: male/female
Strain: Fischer 344
Route of admin.: gavage
Exposure period: 2 years
Frequency of treatment: 5 days/week
Post. obs. period:
Doses: 375 or 750 mg/kg bw for males, 188 or 375 mg/kg bw for females
Result:
Control Group: yes
Method: other
Year: 1988 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: The NTP report concluded that "there was some evidence of carcinogenic activity" in male and femal rats.
Result: 1) 188 mg/kg bw/d:
NOEL;
no effect.
2) 375 mg/kg bw/d:
LOEL;
forestomach, lesions;
mononuclear cell, leukemia, M;
pancreatic acinar cell, adenoma, M;
pituitary, adenoma, F;
adrenal, pheochromocytoma, F.
3) 750 mg/kg bw/d:
forestomach, lesions, M;
adrenal, pheochromocytoma, benign and carcinoma, M.
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
GLP guideline study
05-OCT-2001 (84)

Species: mouse Sex: male/female
Strain: B6C3F1
Route of admin.: oral feed
Exposure period: 2 years
Frequency of treatment: 5 days/week
Post. obs. period:
Doses: 375 or 750 mg/kg bw
Result:
Control Group: yes
Method: other
Year: 1988 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: The NTP report concluded that "there was equivocal evidence for carcinogenic activity" in female mice and no evidence for carcinogenic activity in male mice.
Result: 1) 375 mg/kg bw/d:
liver, adenoma, F;

liver, carcinoma, F.
2) 750 mg/kg bw/d:
no effect.
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
GLP guideline study
05-OCT-2001 (85)

Species: mouse Sex: male/female
Strain: other: Slc: ddY
Route of admin.: oral feed
Exposure period: 20 months
Frequency of treatment: daily
Post. obs. period:
Doses: 30, 120, 480 or 1920 ppm (males: 3.6, 14.7, 57.9 or 289.4 mg/kg bw day; females: 3.6, 13.5, 58.9 or 284.0 mg/kg bw day
Result:
Control Group: yes
Method: other
Year: 1989 GLP: no data
Test substance: other TS: technical grade
Remark: see also chapter 5.4
Result: no significant increase in the tumour incidences
Source: Bayer AG Leverkusen
06-SEP-1994 (68)

Species: mouse Sex: male/female
Strain: other: C57BL/6xC3H/Anf or C57BL/6xAKR hybrids
Route of admin.: other: gavage for 3 weeks and subsequently oral feed for 17 months
Exposure period: 18 months
Frequency of treatment: daily
Post. obs. period:
Doses: 100 mg/kg bw/day (gavage) and 323 ppm (oral feed: 50 mg/kg bw/day)
Result:
Control Group: no data specified
Method:
Year: 1969 GLP: no data
Test substance: other TS: vehicle: 0.5 % gelantine
Remark: Rats were given 100 mg/kg bw/day in a suspension of the vehicle by gavage, beginning when the mice were 7 days of age until 4 weeks of age. After the mice were weaned at 4 weeks of age, the test substance was mixed directly with the diet (no vehicle was used) at a concentration of 323 ppm (50 mg/kg bw/day) for 17 months; 18 animals sex/strain/dose group.
Result: no significant increase in the incidence of tumors after oral administration of 2-mercaptobenzothiazole
Source: Bayer AG Leverkusen
01-SEP-1994 (86) (87)

Species: mouse Sex: male/female
Strain: other: B6C3F1 or B6AKF1 hybrids
Route of admin.: s.c.
Exposure period: see remark
Frequency of treatment: single injection
Post. obs. period: 17 months
Doses: 215 mg/kg bw
Result:
Control Group: other: yes, concurrent vehicle and concurrent no treatment
Method: other: Carcinogenicity Test
Year: 1968 GLP: no data
Test substance: other TS: dissolved in 0.5 % gelantine
Remark: single s.c. injection in nape of neck at 28th day of age; 18 animals/sex/strain/dose and control group.
Result: No significant increase in the incidence of tumors was found.
Source: Bayer AG Leverkusen
01-SEP-1994 (86)

Species: other Sex:
Strain:
Route of admin.:
Exposure period:
Frequency of treatment:
Post. obs. period:
Doses: 18.46 - 110.76 ug/ml
Result:
Control Group:
Method: other: Cell transformation assay
Year: 1982 GLP: yes
Test substance: no data
Result: no increased number of transformed foci
Source: Bayer AG Leverkusen
06-SEP-1994 (77)

5.8 Toxicity to Reproduction

Type:	Two generation study
Species:	rat Sex: male/female
Strain:	Sprague-Dawley
Route of admin.:	oral feed
Exposure Period:	10 weeks before mating, through gestation and lactation until sacrifice
Frequency of treatment:	ad libitum
Premating Exposure Period	
male:	10 weeks
female:	10 weeks
Duration of test:	approximately 88 days past weaning
Doses:	2500, 8750, or 15000 ppm
Control Group:	yes
NOAEL Parental:	< 2500 ppm
NOAEL F1 Offspr.:	< 2500 ppm
NOAEL F2 Offspr.:	< 2500 ppm
Method:	EPA OTS 798.4700
Year:	1991 GLP: yes
Test substance:	other TS: MBT; purity = 98.1%
Remark:	There was no observation of adverse effects on reproductive parameters observed in this study. 2500, 8750, and 15000 ppm = 179, 625, and 1071 mg/kg bw/d conversion number is 14
Result:	1) 2500 ppm: F0; bw, decr, M. 2) 2500 ppm: F1; bw, decr. 3) 2500 ppm: F2; bw, decr. 4) 8750 ppm: F0; bw, decr; food consumption, decr; kidney, decr, weight. 5) 8750 ppm: F1; bw, decr; kidney, decr, weight, M; kidney, brown pigmentation; liver, incr, weight; liver, hepatocellular hypertrophy. 6) 8750 ppm: F2; bw, decr. 7) 15000 ppm: F0; bw, decr; food consumption, decr;

kidney, decr, weight.
8) 15000 ppm:
F1;
bw, decr;
kidney, decr, weight;
kidney, brown pigmentation;
liver, incr, weight;
liver, hepatocellular hypertrophy.
9) 15000 ppm:
F2;
bw, decr.

Reliability: (1) valid without restriction
GLP guideline study

Flag: Critical study for SIDS endpoint

05-OCT-2001 (88)

Type: other
Species: rat Sex: male/female
Strain: Sprague-Dawley
Route of admin.: oral feed
Exposure Period: gestation and lactation and 35-days post-weaning
Frequency of treatment: daily
Duration of test:
Doses: 5000, 10000, or 15000 ppm
Control Group: yes
NOAEL Parental: < 5000 ppm
NOAEL F1 Offspr.: < 5000 ppm
Method: other
Year: 1991 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: This was a rangefinding study.
5000, 10000, and 15000 ppm = 357, 714, and 1071 mg/kg bw/d
conversion number is 14
In the study report, there is reference to two different groups of F0 female rats. The first group, called Group 2, received MBT in the diet at a level of 15000 ppm throughout gestation and lactation. The F1 pups from these dams were exposed to 15000 ppm postweaning. The second group of F0 dams, called Group 3, received MBT in the diet at a level of 15000 ppm during gestation and the first week of lactation, 10000 ppm during the second week of lactation, and 5000 ppm during the third week of lactation. The F1 pups from these dams were exposed to 5000 ppm postweaning.
Result: 1) Group 2 F0 dams:
bw, decreased;
food consumption, decreased.
2) Group 3 F0 dams:
bw, decreased;
food consumption, decreased.
3) F1 pups from Group 2 dams:
bw, decreased.
4) f1 pups from Group 3 dams:
bw, decreased.
Source: Bayer AG Leverkusen

03-NOV-2000 (89)

Type:	other: see Method		
Species:	rat	Sex:	male/female
Strain:	no data		
Route of admin.:	unspecified		
Exposure Period:	see Method		
Frequency of treatment:			
Duration of test:			
Doses:			
Control Group:			
Method:			
Year:		GLP:	
Test substance:	other TS: Captax, purity not noted		
Method:	Trial #1: 5-7 days before mating in males and at estrus state in females. Mating occurred during next estrus. Trial #2: females exposed on day 4 and 11 of pregnancy after mating with untreated males. Females sacficed on 19th day of pregnancy. Obervations: number of yellow bodies (corpora lutea), number of live and dead fetuses, weight and length of fetuses.		
Result:	All accelerators tested had some effect on the development of the fetus.		
Reliability:	(4) not assignable abstract only; translation from Russian		

27-APR-2001 (90)

5.9 Developmental Toxicity/Teratogenicity

Species:	rat	Sex:	female
Strain:	Sprague-Dawley		
Route of admin.:	gavage		
Exposure period:	Day 6-15 of gestation		
Frequency of treatment:	daily		
Duration of test:	up to Day 20 of gestation		
Doses:	300, 1200, or 1800 mg/kg bw/d		
Control Group:	yes		
NOAEL Maternalt.:	= 300 mg/kg bw		
NOAEL Teratogen.:	= 1800 mg/kg bw		
Method:	other		
Year:	1991	GLP:	yes
Test substance:	as prescribed by 1.1 - 1.4		
Remark:	The post-implantation loss was judged to be equivocal since it was not observed at 1200 mg/kg bw/d. There were no other indications that MBT was fetotoxic or teratogenic.		
Result:	1) 300 mg/kg bw/d: PI loss. 2) 1200 mg/kg bw/d: salivation, F; urine staining, F; dark red material around mouth, F.		

3) 1800 mg/kg bw/d:
PI loss;
salivation, F;
urine staining, F;
dark red material around mouth, F;
activity, decr, F;
bw, decr, F;
food consumption, decr, F, Days 6-9.

Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
GLP guideline study
05-OCT-2001 (91)

Species: rabbit Sex: female
Strain: New Zealand white
Route of admin.: gavage
Exposure period: Day 6-18 of gestation
Frequency of treatment: daily
Duration of test: up to Day 29 of gestation
Doses: 150, 300, 600, 1000, or 1500 mg/kg bw/d
Control Group: yes
NOAEL Maternalt.: < 150 mg/kg bw
NOAEL Teratogen.: = 300 mg/kg bw
Method: other
Year: 1991 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: This was a range-finding study. There was no observation of treatment-induced external abnormalities in fetuses.
Result: 1) 150 mg/kg bw/d:
bw, decr, F;
viability, decr, fetal;
bw, decr, fetal.
2) 300 mg/kg bw/d:
bw, decr, F;
viability, decr, fetal;
bw, decr, fetal.
3) 600 mg/kg/bw d:
bw, decr, F;
viability, decr, fetal;
bw, decr, fetal.
4) 1000 mg/kg bw/d:
mortality, F.
5) 1500 mg/kg bw/d:
mortality, F.

Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
05-OCT-2001 (92)

Species: rabbit Sex: female
Strain: New Zealand white
Route of admin.: gavage
Exposure period: Day 6-18 of gestation
Frequency of treatment: daily
Duration of test: up to Day 29 of gestation
Doses: 50, 150, or 300 mg/kg bw/d
Control Group: yes
NOAEL Maternalt.: = 300 mg/kg bw
NOAEL Teratogen.: = 300 mg/kg bw
Method: other
Year: 1991 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: Quality Assurance Statement signed.
There was no indication of fetotoxicity or teratogenicity.
The decreased maternal bw were not statistically significant.
Result: 1) 50 mg/kg bw/d:
no effect.
2) 150 mg/kg bw/d:
NOEL; no effect.
3) 300 mg/kg bw/d:
liver, incr, weight, F;
bw, decr, F.
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
05-OCT-2001 (93)

Species: rat Sex: female
Strain: Sprague-Dawley
Route of admin.: gavage
Exposure period: Day 6-15 of gestation
Frequency of treatment: daily
Duration of test: up to Day 20 of gestation
Doses: 300, 600, 1000, 1500, or 2200 mg/kg bw/d
Control Group: yes
NOAEL Maternalt.: = 1000 mg/kg bw
NOAEL Teratogen.: = 2200 mg/kg bw
Method: other
Year: 1991 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: Quality Assurance Statement signed.
This was a range-finding study. There was no observation of external abnormalities in fetuses.
Result: 1) 300 mg/kg bw/d:
no effect.
2) 600 mg/kg bw/d:
no effect.
3) 1000 mg/kg bw/d:
NOEL;
no effect.

4) 1500 mg/kg bw/d:
bw, decr, F.
5) 2200 mg/kg bw/d:
bw, decr, F;
mortality, F.

Source: Bayer AG Leverkusen
03-NOV-2000 (94)

Species: rat Sex: female
Strain: Sprague-Dawley
Route of admin.: i.p.
Exposure period: Days 1-15 of gestation
Frequency of treatment:
Duration of test:
Doses: 200 mg/kg
Control Group:
NOAEL Maternalt.: 200 mg/kg bw
NOAEL Teratogen.: 200 mg/kg bw
Method: other: Hardin BD, Bond GP, Sikov MR, Andrew FD, Beliles RP, Niemeier RW. (1981) Scan. J. Work Environ. Hlth. 7(S4):66-75
Year: GLP: no data
Test substance: other TS: 2-mercaptobenothiazole; purity not noted
27-APR-2001 (95)

Species: rat Sex: male/female
Strain: no data
Route of admin.: unspecified
Exposure period: see method
Frequency of treatment:
Duration of test:
Doses: not specified
Control Group:
Method:
Year: GLP:
Test substance: other TS: Captax, purity not noted
Method: Trial #1: 5-7 days before mating in males and at estrus state in females. Mating occurred during next estrus.
Trial #2: females exposed on day 4 and 11 of pregnancy after mating with untreated males.

Females sacficed on 19th day of pregnancy.
Obervations: number of yellow bodies (corpora lutea), number of live and dead fetuses, weight and length of fetuses.
Result: All accelerators tested had some effect on the development of the fetus.
Reliability: (4) not assignable
abstract only; translation from Russian
27-APR-2001 (90)

Species: other: chicken embryo
Sex:
Strain:
Route of admin.:
Exposure period:
Frequency of treatment:
Duration of test:
Doses: 0.10, 0.50, 1.0, 1.5, 2.0 umoles/egg
Control Group:
Method:
Year:
GLP:
Test substance: other TS: Vulkacit Mercapto; technical grade
Method: Three day chicken embryos were selected by candling. 5ul of a solution of the test substance in acetone was injected onto the heart of the embryo (Korhonen et al. 1982. Scand. J. Work Environ. Hlth. 8:63). 5ul of acetone was used as a control substance. After 2 days the eggs were candled and dead embryos were discarded. Eggs were again candled every 2 or 3 days; those containing dead embryos were opened and checked for external malformations and the developmental stage. The incubation was terminated 11 days after injection and embryos inspected for survival and external malformations.
Result:

Treatment (umoles/egg)	n=	early deaths	late deaths normal	late deaths malformed	malformed survivors	% affected
0.10	9	0	0	0	1	11%
0.50	30	0	0	0	5	17%
1.0	40	7	0	1	7	38%
1.5	30	6	0	0	6	40%
2.0	30	4	0	0	9	43%

Median effective dose (ED50) = 2.0 umole/egg

27-APR-2001 (96) (97)

5.10 Other Relevant Information

Type: Chemobiokinetics general studies
Remark: 72 % radioactivity excreted in urine and 4 % in feces in 96 hr.
Male and female Fischer 344 rats were dosed orally with 0.592 or 55.5 mg/kg of 14C-labelled MBT, then sacrificed at 8, 24, 72, or 96 hr post-dosing.
Source: Bayer AG Leverkusen
06-NOV-2000 (98)

Type: Chemobiokinetics general studies
Remark: Male and female rats and female guinea pigs were topically exposed to 14C-MBT at approximately 36.1% ug/animal. A separate set of rats were also dosed orally for 14 days with unlabelled MBT at 0.51 mg/kg/day prior to a single dose with 0.503 mg/kg of radiolabelled material. A third set of rats received radiolabelled MBT iv at a dosage of 0.602 mg/kg. Urine excretion of the absorbed dose was > 91 %.

Source: Bayer AG Leverkusen
02-JUN-1994 (99)

Type: Neurotoxicity
Remark: Decreased motor activity was noted.
This study was a rangefinding study. Male and female Sprague-Dawley rats were given MBT by gavage in a corn oil vehicle at dosage levels of 0 or 2750 mg/kg and then observed for 24 hr in a motor activity assessment.
Source: Bayer AG Leverkusen
03-NOV-2000 (100)

Type: Neurotoxicity
Remark: Male and female Sprague-Dawley rats were dosed once by gavage with MBT in a corn oil vehicle at levels of 0, 500, 1250, or 2750 mg/kg bw and then observed for 14 days. Motor activity testing and a functional observational battery were performed.

Based on the findings, it was concluded that the effects seen may be related to an acute, non-specific toxicity without apparent neurotoxicity.
Source: Bayer AG Leverkusen
03-NOV-2000 (101)

Type: Neurotoxicity
Remark: 5000 ppm: NOEL; no effect.
In a three-month study, MBT was administered to Sprague-Dawley rats in the diet at levels of 0, 5000, 15000, or 25000 ppm. [5000, 15000, and 25000 ppm = 357, 2500, and 1786 mg/kg be, conversion number is 14.] Motor activity, functional observational battery, and gross and microscopic evaluations were performed.
Source: Bayer AG Leverkusen
03-NOV-2000 (102)

Type: other
Remark: Revision of chapter 5 (without inquiry): September 94
Source: Bayer AG Leverkusen
06-SEP-1994

Type: other: DNA binding study
Remark: Male and female Fischer 344 rats received a single dose of 375 mg [14C]2-mercaptobenzothiazole/kg bw by gavage; after 8 hours rats were killed, DNA was extracted from liver, adrenals, pituitary gland, pancreas and bone marrow and the amount of DNA associated radioactivity was determined. 2-mercaptobenzothiazole does not significantly bind to DNA from any of the tissues examined. The covalent binding index (CBI) for liver was approximately 1 to 3. The covalent binding indices for the other tissues were below 1. Strong hepatocarcinogens such as dimethylnitrosamine and aflatoxin have CBI values ranging from 6000 to greater than 20000.
Source: Bayer AG Leverkusen
01-SEP-1994 (103)

5.11 Experience with Human Exposure

Remark: A mortality study of workers (2410 employees: 2160 men; 250 women) employed at a manufacturing chemicals plant for the rubber industries in the United Kingdom in the period 1955 - 1986 was performed. The eight hour time weighted average exposures to 2-mercaptobenzothiazole and its derivatives were estimated for different years and for each job and department title. Jobs attracted either zero exposure, very low (0 - 1 mg/m3), low (1 - 2.5 mg/m3), medium (2.5 - 6 mg/m3), or high exposure (6 - 20 mg/m3). The standardized mortality ratios (SMR) for all causes and the SMRs for mortality from cancer were not significantly different from 100. In this study estimated cumulative exposure to 2-mercaptobenzothiazole was not found to be a risk factor.
Source: Bayer AG Leverkusen
01-SEP-1994 (104)

Remark: Mortality trends for 1059 production workers at a rubber chemical plant in Nitro, West Virginia (USA) during 1955 - 1987 were examined to find whether they had increased mortality from cancer associated with exposure to 2-mercaptobenzothiazole. This chemical has been manufactured at the plant since 1935. Analyses were conducted on 2-mercaptobenzothiazole exposed employees by cumulative exposure and time since first exposure, and were also stratified by past assignment to p-aminobiphenyl-related departments; p-aminobiphenyl is a potent bladder carcinogen, that was used at the plant between 1935 and 1955. An excess of bladder cancer was seen in 2-mercaptobenzothiazole workers who also had job assignments with exposure to p-aminobiphenyl. In workers without a job assignment with exposure to p-aminobiphenyl, there were no associations between exposure to 2-mercaptobenzothiazole and increased rates of most malignant neoplasms. The standardized mortality ratio (SMR) for bladder cancer was raised, although there were too few deaths to evaluate trends exposure category. There were no deaths from bladder cancer among 2-mercaptobenzothiazole workers hired after the end of p-aminobiphenyl use at the plant although only 0.03 deaths were expected.
Source: Bayer AG Leverkusen
02-SEP-1994 (105)

(1) CRC Handbook of Chemistry and Physics. 80th edition (1999-2000) David R. Lide, ed. CRC Press, New York. p3-80, No. 2866.

(2) The Merck Index Eleventh Edition - 1989.

(3) Monsanto manufacturing data.

(4) The Merck Index Eleventh Edition - 1989. Nine-volume 2nd edition of the CRC handbook of data on organic compounds.

(5) Monsanto study number SR-85-X017.

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

(7) Monsanto report number SR-85-X017.

(8) Environ Toxicol Chem 11:1153-68

(9) Bayer manufacturing data.

(10) Springborn Laboratories Report # 89-9-3094. Jointly sponsored through the Chemical Manufacturer's Association as part of a TSCA Section 4 test rule.

(11) Brownlee, B.G. J.H. Carey, G.A. MacInnis and I.T. Pellizzari (1992), Aquatic environmental chemistry of 2-(thiocyanomethylthio) benzothiazole and related benzothiazoles, Environmental Toxicology and Chemistry 11, 1153-1168.

(12) Parkanyi, C. and A.O. Abdelhamid (1985), Photodegradation of pesticides: photolysis of 2-mercaptobenzothiazole and 2-mercaptobenzimidazole, Heterocycles 23(11), 2917-2926.

(13) Mitchell, L.C. (1961), The effect of ultraviolet light (2537A) on 141 pesticide chemicals by paper chromatography, Journal Association of Official Agricultural Chemistry 44:643-712.

(14) Monsanto report SR-85-0017

(15) Monsanto report AB-85-X016.

(16) Monsanto Study No. AB-84-X134. Analytic Bio-Chemistry Labs (1984)

(17) Keith, L.H. (1976), Identification of organic compounds in unbleached treated Kraft paper mill wastewaters, Environmental Science and Technology 10(6), 555-564.

(18) Springborn Laboratories Report # 89-9-3086. Jointly sponsored through the Chemical Manufacturer's Association as part of a TSCA Section 4 test rule.

(19) Monsanto Study #AN6405; August 19, 1980

(20) Springborn Laboratories Report # 89-9-3087. Jointly sponsored through the Chemical Manufacturer's Association as part of a TSCA Section 4 test rule.

(21) Biodegradation and Bioaccumulation Data of Existing Chemicals Based on the CSCL Japan, Compiled under the Supervision of Chemical Products Safety Division, Basic Industries Bureau MITI, Ed. by CITI, October 1992. Published by Japan Chemical Industry Ecology-Toxicology & Information Center

(22) Monsanto report MO-92-9056

(23) Monsanto report SR-85-0017.

(24) Tomlinson, T.G., A.G. Boon and C.N.A. Trotman (1966), Inhibition of nitrification in the activated sludge process of sewage disposal, Journal of Applied Bacteriology, 29(2), 266-291.

(25) Williams, G.R. (1984), The Effect of both powdered and liquid rubber additives on the growth of soil microorganisms, International Biodeterioration 20(3),173-5.

(26) Kondo, M., T. Nishihara, T. Shimamoto, T. Koshiwaka, T. Ii O, R. Sawamura,and K. Tanaka (1988A), Biodegradation Test of Chemicals by Cultivation Method, Eisei Kagaku 34,188-195.

(27) Thom, N.S. and A.R. Agg (1975), The breakdown of synthetic organic compounds in biological processes, Proceedings of the Royal Society London B. 189, 347-357.

(28) M. Kawasaki (1980), Experiences with the test scheme under the chemical control law of Japan: an approach to structure-activity correlations, Ecotoxicology and Environmental Safety 4, 444-454.

(29) Hashimoto, K., Y. Sasaki, Y. Ohara, and T. Matsuzawa (1978), Absorption, distribution and excretion of 2-mercaptobenzothiazole in carp, Bulletin Japanese Society of Scientific Fisheries 44(6), 623-629.

(30) Sasaki, S. (1979), The scientific aspects of the chemical substance control law in Japan, in Aquatic Pollutants: Transformation and Biological Effects. Hutzinger, O. et al (eds). Oxford: Pergamon Press. pp283-298.

(31) Monsanto report AB-79-0315

(32) Bayer AG report

(33) Monsanto report BN-76-0169

(34) Sollmann, T. (1949), Correlation of the aquarium goldfish toxicities of some phenols, quinones, and other benzene derivatives with their inhibition of autooxidative reactions, Journal General Physiology 32, 671-679.

Verschueren, K. (1983), Handbook of Environmental Data on Organic Chemicals. Van Nostrand Reinhold Company, Inc. NY.

(35) Monsanto report SR-83-X062

(36) Monsanto report AB-79-0314

(37) (2-Mercaptobenzothiazole (ROKON)) - Acute Toxicity to Daphnids (Daphnia magna) under Static Conditions (Final Report), EPA/OTS; Doc #86-920000843 (1992)

(38) Monsanto report BN-79-0313

(39) Yoshioka, Y. (1985), Testing for the toxicity of chemicals with Tetrahymena pyriformis, The Science of the Total Environment 43, 149-157.

(40) Santodonato, J., L.N. Davis, P.H. Howard and J. Saxena (1976), Investigation of selected potential environmental contaminants: mercaptobenzothiazoles, EPA-560/2-76-006.

(41) Brown, S.L., F.Y. Chan, J.L. Jones (1975), Research program on hazard priority ranking of manufactured chemicals (chemicals 41-60), Stanford Research Institute. Menlo Park, CA 191 NSF-RA-E-75-190C.

(42) Springborn Laboratories Report # 89-9-3083. Jointly sponsored through the Chemical Manufacturer's Association as part of a TSCA Section 4 test rule.

(43) Springborn Laboratories Report # 89-9-3082. Jointly sponsored through the Chemical Manufacturer's Association as part of a TSCA Section 4 test rule.

(44) Monsanto report Y-75-0237

(45) Monsanto report Y-73-0288

(46) Guess WL and O'Leary RK. Toxicol and Appl Pharm. 14: 221-231 (1969)

(47) McCormick, WE. Rubber Chemistry and Tehnology 44(2): 512-530. (1971)

(48) Monsanto report SA-55-0074

(49) Industrial Bio-TEST-Laboratories Inc. (1977): IBT No. 8562-10075
In: Ciba Geigy Corp. (1985): NTIS/OTS 0206754

(50) DOW Chemical Co. (1961): Results of range finding toxicological tests on 2 mercaptobenzothiazole (Captex) cited in: Syracuse Research Corporation (1985): Technical Support Document 2-Mercaptobenzothiazole

(51) Basketter, D.A. et al. (1993): Food Chem. Toxicol. 31, 63 - 67

(52) Wang, X. and Suskind, R.R. (1988), Comparative studies of the sensitization potential of morpholine, 2-mercaptobenzothiazole and 2 of their derivatives in guinea pigs, Contact Dermatitis, 19, 11-15.

(53) Basketter, D.A., Scholes, E.W. (1992): Food Chem. Toxicol. 30, 65 - 69

(54) Scholes, E.W. et al. (1992): J. Appl. Toxicol. 12, 217 - 222

(55) Magnusson, B. and Kligman, A.M. (1970), Allergic Contact Dermatitis in the Guinea Pig, C.C. Thomas, ed., Springfield, IL.

(56) Magnusson, B. and Kligman, A.M. (1968), The identification of contact allergens by animal assay, the guinea pig maximization test method, Journal of Investigative Dermatology, 52, 268-276.

(57) Kaniwa, M.-A. et al. (1992): Contact Dermatitis 27, 166 - 173

(58) Ziegler, V. et al. (1972): Allergie und Immunologie 18, 203 - 208

(59) Ikarashi, Y. et al (1993), Evaluation of contact sensitivity of rubber chemicals using the murine local lymph node assay, Contact Deramtitis, 28, 77-80.

(60) Kammueller, M.E. et al. (1989): Int. J. Immunopharmac. 11, 293 - 300

(61) Monsanto report SH-76-0005

(62) Monsanto report ML-87-0068

(63) Bourrinet, P. et al. (1979): J. Pharm. Belg. 34, 21 - 26

(64) National Toxicology Program report NTP TR 332.

(65) Physiolological research Laboratories 78-60-106002 (1981)

(66) Monsanto report ML-88-0426

(67) Monsanto Report MSL-8968

(68) Ogawa, Y. et al. (1989): Bull. Natl. Inst. Hyg. Sci. 107, 44 - 50

(69) BF Goodrich Study No. 22 (1984)

(70) Monsanto report PK-86-9005. Jointly sponsored through the Chemical Manufacturer's Association, study No. PH 301-CMA-001-83.

(71) WTR International Work Group on the Toxicology of Rubber. Central Toxicology Laboratory Study No. CTL/5548. (1997)

(72) Monsanto report BO-76-0177

(73) Szybalski, W. (1958): Ann. N.Y. Acad. Sci. 76, 475 - 489

(74) Donner, M. et al. (1983): Scand. J. Work Environ. Health 9, Suppl. 2, 27 - 37

(75) Monsanto report PK-86-9006. Jointly sponsored through the Chemical Manufacturer's Association, study No. PH 314-CMA-001-83

(76) Monsanto report BO-78-0240

(77) Litton Bionetics, Inc. (1985): LBI Project No. 20989

(78) Myhr, B. et al. (1990): Environ. Mol. Mutagen. 16, Suppl. 18, 138 - 144, 156

(79) Monsanto report LB-86-9004. Jointly sponsored study through the Chemical Manufacturer's Association. Litton Bionetics, Inc. Project No. 20989.

(80) Monsanto report SB-91-9705. SLS Study No. 3205.6 Jointly sponsored by the Chemical Manufacturer's Association as part of a TSCA Section 4 test rule study. Springborn Laboratories Study No. 3205.5, 3205.6, 3205.7

(81) Monsanto report PK-86-9007. Jointly sponsored through the Chemical Manufacturer's Association, study No. PH 309A-CMA-001-83.

(82) Monsanto Environmental Health Lab Study No. 87134 (1988)

(83) Revazova, Y.A. (1968): Toksikol. Nov. Khim. Veshchestv, Vnedryaemykh Rezin. Shinnuyu Prom., 196 - 203 In: Chemical Abstr. 71, 47071e (1969)

(84) National Toxicology Program report NTP TR 332; NIH Publication No. 88-2588

(85) Monsanto report XX-86-9079. Jointly sponsored through the Chemical Manufacturer's Association as part of a TSCA Section 4 test rule.

(86) Bionetics Research Laboratories, Inc. (1968): NTIS/PB 223159

(87) Innes, J.R.M. et al. (1969): J. Natl. Cancer Inst. 42, 1101 - 1114

(88) Springborn Laboratories, study No. 3205.5, Jointly sponsored through the Chemical Manufacturer's Association as part of a TSCA Section 4 test rule.

(89) Monsanto report SB-91-9708. Jointly sponsored through the Chemical Manufacturer's Association as part of a TSCA Section 4 test rule SLS Study No. 3205.7

(90) Alexandrov, SE. (1974) Tezisy Dokl. Nauchn. Sess. Khim. Teknol. Org. Soedin. Sery Sernistykh Neftei. 13:98-99

(91) Monsanto report SB-91-9702. Jointly sponsored through the Chemical Manufacturer's Association as part of a TSCA Section 4 test rule. Rodwell, D.E. et al (1990), Developmental toxicity study of 2-mercaptobenzothiazole (MBT) in two species, Teratology, p. 587 (abstract).

(92) Monsanto report SB-91-9703. Jointly sponsored through the Chemical Manufacturer's Association as part of a TSCA Section 4 test rule, SLS study No.3205.1

(93) Monsanto report SB-91-9704. Jointly sponsored through the Chemical Manufacturer's Association as part of a TSCA Section 4 test rule. SLS Study No. 3205.4 Rodwell, D.E. et al (1990), Developmental toxicity study of 2-mercaptobenzothiazole (MBT) in two species, Teratology, p. 587 (abstract).

(94) Monsanto report SB-91-9701. Jointly sponsored through the Chemical Manufacturer's Association as part of a TSCA Section 4 test rule, SLS Study No. 3205.2

(95) Hardin BD, Bond GP, Sikov MR, Andrew FD, Beliles RP, Niemeier RW. (1981) Scan. J. Work Environ. Hlth. 7(S4):66-75

(96) Korhonen A, Hemminki K, Vainio H. (1982) Arch. Environ. Contam. Toxicol. 11:753-759.

(97) Korhonen A, Hemminki K, Vainio H. (1983) Scan. J. Work Environ. Hlth. 9:115-119

(98) Monsanto report SR-92-9055. Jointly sponsored through the Chemical Manufacturers Association as part of U. S. EPA TSCA Section 4 test rule.

(99) El Dareer, S.M., et al (1989), Disposition of 2-mercaptobenzothiazole and 2-mercaptobenzothiazole disulfide in rats dosed intravenously, orally, and topically and in guinea pigs dosed topically, Journal of Toxicology and Environmental Health, 27, 65-84.

(100) Monsanto Study BR-91-9707. Jointly sponsored through the Chemical Manufacturers Association as part of U. S. EPA TSCA Section 4 test rule, Project No. 83800

(101) Monsanto Study BR-91-9706. Jointly sponsored through the Chemical Manufacturers Association as part of U. S. EPA TSCA Section 4 test rule, Project No. 83801.
Bannister, R.M. et al (1991), Acute and subchronic neurotoxicity evaluation of 2-mercaptobenzothiazole (MBT) in rats, The Toxicologist, 11, 117 (Abstract).

(102) Monsanto Study XX-90-9513. Jointly sponsored through the Chemical Manufacturers Association as part of U. S. EPA TSCA Section 4 test rule.
Bannister, R.M. et al (1991), Acute and subchronic neurotoxicity evaluation of 2-mercaptobenzothiazole (MBT) in rats, The Toxicologist, 11, 117 (Abstract).

(103) Brewster, D.W. et al. (1989): Biochem. Biophys. Res. Commun. 165, 342 - 348

(104) Sorahan, T., Pope, D. (1993): Br. J. Ind. Med. 50, 998 - 1002

(105) Strauss, M.E. et al. (1993): Br. J. Ind. Med. 50, 888 - 893

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: 155-04-4
CAS No.	155-04-4
EINECS Name	zinc di(benzothiazol-2-yl) disulphide
EINECS No.	205-840-3
Molecular Formula	C7H5NS2.1/2Zn

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

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

Memo: Rubber and Plastics Additives (RAPA) HPV Panel

Printing date: 09-OCT-2001
Revision date:
Date of last Update: 09-OCT-2001

Number of Pages: 29

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: American Chemistry Council, Rubber and Plastic Additives (RAPA) HPV Panel
Street: 1300 Wilson Boulevard
Town: VA 22209 Arlington
Country: United States
Phone: 703-741-5600

09-OCT-2001

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

08-OCT-2001

Type: cooperating company
Name: Ciba Specialty Chemicals Corporation
Country: United States

09-OCT-2001

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

09-OCT-2001

Type: cooperating company
Name: Flexsys America, L.P.
Town: 0444
Country: United States

09-OCT-2001

Type: cooperating company
Name: Noveon, Inc (formerly BF Goodrich)
Country: United States

09-OCT-2001

Type: cooperating company
Name: R.T. Vanderbilt Company, Inc.
Country: United States

09-OCT-2001

Type: cooperating company
Name: The Goodyear Tire & Rubber Company
Country: United States

09-OCT-2001

Type: cooperating company
Name: The Lubrizol Corporation
Country: United States

09-OCT-2001

Type: cooperating company
Name: UOP, LLC.
Country: United States

09-OCT-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: 97 % w/w
13-OCT-1999

1.1.0 Details on Template
-

1.1.1 Spectra
-

1.2 Synonyms

2-benzothiazole, zinc salt
13-OCT-1999

2-mercaptobenzothiazole, zinc salt
13-OCT-1999

Vulkacit ZM
13-OCT-1999

ZMBT
13-OCT-1999

1.3 Impurities

CAS-No: 149-30-4
EINECS-No: 205-736-8
EINECS-Name: benzothiazole-2-thiol
Contents: 11 - 16 % w/w
13-OCT-1999

CAS-No:
EINECS-No:
EINECS-Name: inorganics (NaCl, NaSO4)
Contents: <= .5 % w/w
13-OCT-1999

CAS-No: 7732-18-5
EINECS-No: 231-791-2
EINECS-Name: water
Contents: <= .3 % w/w
13-OCT-1999

1.4 Additives

CAS-No:
EINECS-No:
EINECS-Name: emulgator
Contents: 0 - .5 % w/w
13-OCT-1999

1.5 Quantity
-

1.6.1 Labelling
-

1.6.2 Classification
-

1.7 Use Pattern

Type: type
Category: Non dispersive use
13-OCT-1999

Type: industrial
Category: Polymers industry
13-OCT-1999

Type: use
Category: Vulcanizing agents
13-OCT-1999

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:	233.3 degree C
Method:	other: MPBPWIN (v1.31)
Year:	1999
GLP:	no
Testsubstance:	other TS: molecular structure
Result:	Melting Point: 349.84 deg C (Adapted Joback Method) Melting Point: 204.21 deg C (Gold and Ogle Method) Mean Melt Pt : 277.03 deg C (Joback; Gold,Ogle Methods) Selected MP: 233.34 deg C (Weighted Value)
Reliability:	(2) valid with restrictions Accepted calculation method
Flag:	Critical study for SIDS endpoint

09-OCT-2001 (1)

Value:	310 degree C
Method:	other: historical data

09-OCT-2001 (2)

Value:	340 degree C
Method:	other: historical data
Flag:	Critical study for SIDS endpoint

25-APR-2001 (3)

2.2 Boiling Point

Value:	544.4 degree C at 1013 hPa
Method:	other: 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

09-OCT-2001 (1)

2.3 Density

Type:	
Value:	ca. 1.7 g/cm3
Source:	Bayer AG Leverkusen

26-SEP-1994 (2)

2.3.1 Granulometry

-

2.4 Vapour Pressure

Value: .0000000000155 hPa at 25 degree C
Method: other (calculated): MPBPWIN (v1.31) Modified Grain Method
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Result: Vapor Pressure Estimations (25 deg C):
(Using BP: 544.40 deg C (estimated))
(Using MP: 233.34 deg C (estimated))
VP: 2.94E-014 mm Hg (Antoine Method)
VP: 1.16E-011 mm Hg (Modified Grain Method)
VP: 3.75E-011 mm Hg (Mackay Method)
Selected VP: 1.16E-011 mm Hg (Modified Grain Method)
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
09-OCT-2001 (1)

2.5 Partition Coefficient

log Pow: 5.016 at 25 degree C
Method: other (calculated): KOWWIN Program (v1.65)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
09-OCT-2001 (1)

2.6.1 Water Solubility

Value: 90.9 mg/l at 20 degree C
Source: Bayer AG Leverkusen
Flag: Critical study for SIDS endpoint
09-OCT-2001 (4)

Value: .01275 at 25 degree C
Method: other: WSKOW (v1.36)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Result: Log Kow (estimated) : 5.02
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: 5.02

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW +
Correction (used when Melting Point NOT available)

Correction(s):	Value

PAH Type -1.110

Log Water Solubility (in moles/L) : -7.494
Water Solubility at 25 deg C (mg/L): 0.01275

Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
09-OCT-2001 (1)

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: ca. .0000000000902585 cm3/(molecule * sec)
Degradation: ca. 50 % after 1.4 hour(s)
Method: other (calculated):AOPWin (v1.88) Estimations Program
Year: 1999 GLP:
Test substance: other TS: chemical structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
09-OCT-2001 (1)

3.1.2 Stability in Water

Type: abiotic
Method:
Year: GLP:
Test substance:
Remark: See IUCLID documents on CAS# 149-30-4
09-OCT-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	0.132	2.84	1000	3.12e-015
Water	19.1	900	1000	2.77e-015
Soil	55.9	900	1000	9.35e-017
Sediment	24.9	3.6e+003	0	1.87e-015

Persistence Time: 864 hr
Reaction Time: 1.05e+003 hr

Advection Time: 4.78e+003 hr
Percent Reacted: 81.9
Percent Advected: 18.1
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
09-OCT-2001 (1)

3.3.2 Distribution

Media: air - biota - sediment(s) - soil - water
Method: other (calculation): fugacity level III
Year: 1999
Result:

Compartment	Conc.(%)	Half-life(hr)	Emissions(kg/hr)
Air	0.104	2.84	1000
Water	17.4	0.00148	1000
Soil	72.1	0.00148	1000
Sediment	10.4	0.00148	0

Reliability: (2) valid with restrictions
13-OCT-1999 (5)

3.4 Mode of Degradation in Actual Use
-

3.5 Biodegradation

Type: aerobic
Inoculum:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID documents on CAS# 149-30-4
09-OCT-2001

3.6 BOD5, COD or BOD5/COD Ratio

B O D 5

BOD5: 0 mgO2/l

Remark: no degradation
Source: Bayer AG Leverkusen
08-NOV-1993 (4)

3.7 Bioaccumulation

Species: other: calculation
Exposure period:
Concentration:
BCF: 1453
Elimination:
Method: other: BCF Program (v2.13)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Result: Log Kow (estimated) : 5.02
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 5.02

Equation Used to Make BCF estimate:
Log BCF = 0.77 log Kow - 0.70

Estimated Log BCF = 3.162 (BCF = 1453)
Reliability: (2) valid with restrictions
Accepted calculation method
09-OCT-2001 (1)

3.8 Additional Remarks

-

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: static
Species: Leuciscus idus (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
LC0: 10
LC100: 50
Method: other: Bestimmung der akuten Wirkung von Stoffen auf Fische. Arbeitskreis "Fischtest" im Hauptausschuss "Detergentien" (15.10.73)
Year: 1975 GLP: no
Test substance:
Remark: direct weight
Source: Bayer AG Leverkusen
Flag: Critical study for SIDS endpoint
09-OCT-2001 (4)

Type: other: calculation
Species: other: fish
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: .427
Method: other: (calculated) ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
09-OCT-2001 (1)

Type: other: calculation
Species: other: fish
Exposure period: 14 day
Unit: mg/l Analytical monitoring: no
LC50: 1.251
Method: other: (calculated) ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
09-OCT-2001 (1)

4.2 Acute Toxicity to Aquatic Invertebrates

Type: other: calculated
Species: Daphnia sp. (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: .564
Method: other: (calculated) ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
09-OCT-2001 (1)

Type:
Species:
Exposure period:
Unit: Analytical monitoring:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID documents on CAS# 149-30-4
09-OCT-2001

Type: other: calculated
Species: Mysidopsis bahia (Crustacea)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
NOEC: .014
Method: other: (calculated) ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
09-OCT-2001 (1)

Type: other: calculated
Species: Daphnia sp. (Crustacea)
Exposure period: 16 day
Unit: mg/l Analytical monitoring: no
EC50: .108
Method: other: (calculated) ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
09-OCT-2001 (1) (1)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: other algae: green algae
Endpoint: growth rate
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: .42
ChV : .24
Method: other: (calculated) ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
09-OCT-2001 (1)

Species:
Endpoint:
Exposure period:
Unit: Analytical monitoring:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID documents on CAS# 149-30-4
09-OCT-2001

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: 1220
EC05 : 70
Method: ISO 8192 "Test for inhibition of oxygen consumption by activated sludge"
Year: 1990 GLP: yes
Test substance:
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
GLP guideline study
09-OCT-2001 (4)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

Species: other: fish
Endpoint:
Exposure period: 30 day
Unit: mg/l Analytical monitoring: no
LLC: .09
Method: other: (calculated) ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
09-OCT-2001 (1)

4.5.2 Chronic Toxicity to Aquatic Invertebrates
-

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms

Type: other: calculated
Species: Eisenia fetida (Worm (Annelida), soil dwelling)
Endpoint:
Exposure period: 14 day
Unit: other: mg/l
LC50: 287.457
Method: other: (calculated) ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
09-OCT-2001 (1)

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:	20
Vehicle:	other: propylene glycol
Value:	> 10000 mg/kg bw
Method:	
Year:	GLP: no data
Test substance:	other TS: Vulcafor ZMBT; purity not noted
Method:	The test material was given as a 33% (w/v) suspension in propylene glycol to groups of 10 males and 10 females in a single dose of 30 ml/kg bw (10g test material/kg bw). The rats received feed and water ad libitum during the 14 day observation period. The rats were observed for intoxication and mortality. All animals were necropsied.
Remark:	mortality: 4/20 died. Within a few minutes of dosing, all rats showed sluggishness, followed by loss of conciousness. Two males and two females died between 2 and 15 hours after treatment. After 24 hours, the survivors recovered and looked healthy during the 14 day observation period. Macroscopic examination of the survivors did not reveal treatment-realted gross alterations.
Reliability:	(2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag:	Critical study for SIDS endpoint

09-OCT-2001 (6)

Type:	LD50
Species:	rat
Strain:	
Sex:	
Number of Animals:	
Vehicle:	
Value:	> 5000 mg/kg bw
Method:	other
Year:	GLP: no data
Test substance:	other TS: commercial grade
Remark:	mortality: 0/20

25-APR-2001 (7) (8)

Type: LD50
Species: rat
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: = 7500 mg/kg bw
Method: other
Year: GLP: no data
Test substance: other TS: no data
25-APR-2001 (9)

5.1.2 Acute Inhalation Toxicity

Type:
Species:
Strain:
Sex:
Number of
Animals:
Vehicle:
Exposure time:
Value:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID documents on CAS #149-30-4 and #2492-26-4
09-OCT-2001

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rabbit
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: > 7940 mg/kg bw
Method: other
Year: GLP: no data
Test substance: other TS: no data
Remark: mortality: 0/2
Source: Bayer AG Leverkusen
Reliability: (3) invalid
Documentation insufficient for assessment
09-OCT-2001 (9)

Type: other
Species:
Strain:
Sex:
Number of
Animals:
Vehicle:
Value:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID documents on CAS #149-30-4 and #2492-26-4
09-OCT-2001

5.1.4 Acute Toxicity, other Routes

Type: other: approx. LD50
Species: mouse
Strain:
Sex:
Number of
Animals:
Vehicle:
Route of admin.: i.p.
Value: 200 - 300 mg/kg bw
Method: no data
Year: GLP: no data
Test substance: no data
Source: Bayer AG Leverkusen
21-SEP-1994 (10)

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: other: 24 hours exposure; 7-d observation period
Year: GLP: no data
Test substance: other TS: no data
Remark: scores in accordance with Federal Hazardous Substances Act, 21 CFR, § 191.12 (1964)
Source: Bayer AG Leverkusen
22-SEP-1994 (9)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result: not irritating
EC classificat.:
Method: other: 24 hours exposure; 7-d observation period
Year: GLP: no data
Test substance: other TS: no data
Remark: scores in according to the method of Draize
Source: Bayer AG Leverkusen
21-SEP-1994 (11)

5.2.2 Eye Irritation

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of
Animals:
Result: not irritating
EC classificat.:
Method: other: 100 mg was placed into the conjunctival sac of 6 rabbits; 7-d observation period
Year: GLP: no data
Test substance: other TS: no data
Remark: scores in accordance with FDA scoring scale, Fed. Reg. 28 (119), 5582, 1963
Source: Bayer AG Leverkusen
21-SEP-1994 (11)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of
Animals:
Result: not irritating
EC classificat.:
Method: other: 100 mg was placed into the conjunctival sac of 6 rabbits; 7-d observation period
Year: GLP: no data
Test substance: other TS: no data
Remark: scores in accordance with Federal Hazardous Substances Act, 21 CFR, § 191.12 (1964): 1.7/110.0
Source: Bayer AG Leverkusen
22-SEP-1994 (9)

5.3 Sensitization

Type:	Patch-Test
Species:	human
Number of Animals:	
Vehicle:	
Result:	
Classification:	
Method:	other
Year:	GLP: no data
Test substance:	other TS: 1 % in Eucerin anhydric
Remark:	result: 2/5 patients with a rubber eczema were positive with Zn-MBT among others
Source:	Bayer AG Leverkusen

22-SEP-1994 (12)

Type:	Patch-Test
Species:	human
Number of Animals:	
Vehicle:	
Result:	
Classification:	
Method:	other
Year:	GLP: no data
Test substance:	other TS: 1 % pet.
Remark:	result: 15/17 subjects allergic to MBT were positive with Zn-MBT
Source:	Bayer AG Leverkusen

21-SEP-1994 (13)

5.4 Repeated Dose Toxicity

Species:		Sex:	
Strain:			
Route of admin.:			
Exposure period:			
Frequency of treatment:			
Post. obs. period:			
Doses:			
Control Group:			
Method:			
Year:		GLP:	
Test substance:			
Remark:	See IUCLID documents on CAS# 149-30-4		

09-OCT-2001

5.5 Genetic Toxicity 'in Vitro'

Type: Bacterial gene mutation assay
System of testing: S. typhimurium TA 98, TA 100, TA 1535, TA 1537
Concentration: up to 3000 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: GLP: no
Test substance: no data
Source: Bayer AG Leverkusen
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
09-OCT-2001 (14)

Type: Bacterial gene mutation assay
System of testing: S. typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration: up to 500 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: GLP:
Test substance: no data
Source: Bayer AG Leverkusen
09-OCT-2001 (15)

Type: Gene mutation in Saccharomyces cerevisiae
System of testing: strain D4
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: GLP:
Test substance: no data
Source: Bayer AG Leverkusen
09-OCT-2001 (15)

Type: Bacterial gene mutation assay
System of testing: S. typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration: up to 3000 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result:
Method: other: no data
Year: GLP: no data
Test substance: no data
Remark: result: weakly positive (+ S9-mix)
Source: Bayer AG Leverkusen
09-OCT-2001 (16)

Type:
System of testing:
Concentration:
Cytotoxic Conc.:
Metabolic activation:
Result:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID documents on CAS #149-30-4 and #2492-26-4
09-OCT-2001

Type: Ames test
System of testing: S. typhimurium
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
30-OCT-2000 (17)

Type: Bacterial gene mutation assay
System of testing: S. typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: GLP:
Test substance: no data
Remark: substance was not toxic for the test strains in higher concentrations

Source: Bayer AG Leverkusen
21-SEP-1994 (18)

5.6 Genetic Toxicity 'in Vivo'

Type:
Species: Sex:
Strain:
Route of admin.:
Exposure period:
Doses:
Result:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID documents on CAS# 149-30-4
09-OCT-2001

5.7 Carcinogenicity

Species: mouse Sex: male/female
Strain: other: B6C3F1 and B6AKF1
Route of admin.: other: a single s.c. injection at 28th day of age
Exposure period:
Frequency of treatment: once
Post. obs. period: 18 months
Doses: 1000 mg/kg
Result: negative
Control Group: yes, concurrent vehicle
Method: other
Year: GLP: no data
Test substance: other TS: no data
Remark: maximal tolerated doses were given (no further information)
Result: Zn-MBT did not cause a significant increase in tumors
Source: Bayer AG Leverkusen
09-OCT-2001 (19)

Species: mouse Sex: male/female
Strain: other: B6C3F1 and B6AKF1
Route of admin.: other: gavage (days 7-28 of age) and in the diet (after 28 days of age)
Exposure period: 18 months
Frequency of treatment: daily
Post. obs. period: no
Doses: 1000 mg/kg (gavage) 3385 ppm (diet)
Result:
Control Group: yes, concurrent vehicle
Method: other
Year: GLP: no data
Test substance: other TS: no data
Remark: maximal tolerated doses were given (no further information)
Result: Zn-MBT did not cause a significant increase in tumors
Source: Bayer AG Leverkusen
22-SEP-1994 (19) (20)

5.8 Toxicity to Reproduction

Type:
Species: Sex:
Strain:
Route of admin.:
Exposure Period:
Frequency of treatment:
Duration of test:
Doses:
Control Group:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID documents on CAS# 149-30-4
09-OCT-2001

5.9 Developmental Toxicity/Teratogenicity

Species: other Sex:
Strain:
Route of admin.:
Exposure period:
Frequency of treatment:
Duration of test:
Doses:
Control Group:
Method: other
Year: GLP:
Test substance: no data
Method: three day White Leghorn chicken embryos were injected by the dropping of the chemical into the air chamber of the egg.
Result: even the highest doses (1.0 umoles/egg) did not produce effects above the level of the acetone background
Source: Bayer AG Leverkusen
Reliability: (2) valid with restrictions
09-OCT-2001 (21) (22)

Species: Sex:
Strain:
Route of admin.:
Exposure period:
Frequency of treatment:
Duration of test:
Doses:
Control Group:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID documents on CAS# 149-30-4
09-OCT-2001

5.10 Other Relevant Information
-

5.11 Experience with Human Exposure
-

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

(2) Safety data sheet Vulkacit ZM, Bayer AG

(3) Monsanto MSDS. May, 1975

(4) Bayer AG data

(5) Syracuse Research Corporation

(6) de Groot, A.P., CIVO TNO (1975)

(7) Sumitomo Chemical Co. data, December 1, 1977

(8) Uniroyal MSDS. Sept. 1985.

(9) Younger Laboratories data, Project No. Y-74-288, January 28, 1975, NTIS/OTS0206761, Doc. I.D. 878215076

(10) Doull, J. AD-277-689, April 1962

(11) van Beek, L., CIVO TNO Report No. R 5042, June 1976

(12) Bandmann, H.-J., Der Hautarzt 7 (9), 419-421 (?)

(13) Foussereau, J. et al., Contact Dermatitis 9, 514-516 (1983)

(14) Goodyear data, Laboratory Report No. 80-4-3, June 25, 1980

(15) Litton Bionetics data, Project No. 2683, July, 1977, NTIS/OTS0206761; Doc. I.D. 878215077

(16) Sumitomo Chemical Co. data, September 24, 1981

(17) Hedenstedt A, Rannung U, Ramel C, Wachtmeister CA Mutat. Res. (Netherlands) 68(4): 313-325 (1979)

(18) Rannug, A. et al., Prog. Clin. Biol. Res. 141, 407-419 (1984)

(19) Bionetics Research Labs. prepared for NCI, PB-223 159, August 1968

(20) Innes, J.R.M. et al., J. National Cancer Inst., 42 1101-1114 (1969)

(21) Korhonen, A. et al., Archro. Envinm. Contam. Toxicol. 11, 753-759 (1982)

(22) Korhonen, A. et al., Scand. J. Work Environ. Health 9, 115-119 (1983)

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: 2492-26-4
CAS No.	2492-26-4
EINECS Name	sodium benzothiazol-2-yl sulphide
EINECS No.	219-660-8
TSCA Name	2(3H)-Benzothiazolethione, sodium salt
Molecular Formula	C7H5NS2.Na

Producer Related Part	
Company:	
Creation date:	13-OCT-1999

Substance Related Part	
Company:	
Creation date:	13-OCT-1999

Memo:	Rubber and Plastics Additives (RAPA) HPV Panel

Printing date:	09-OCT-2001
Revision date:	
Date of last Update:	09-OCT-2001

Number of Pages:	37

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: American Chemistry Council, Rubber and Plastic Additives Panel (RAPA)
Street: 1300 Wilson Boulevard
Town: 22209 Arlington, VA
Country: United States
Telefax: 703-741-6091

08-OCT-2001

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

08-OCT-2001

Type: cooperating company
Name: Ciba Specialty Chemicals Corporation
Country: United States

08-OCT-2001

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

08-OCT-2001

Type: cooperating company
Name: Flexsys America L.P.
Country: United States

08-OCT-2001

Type: cooperating company
Name: Noveon, Inc (formerly BF Goodrich)
Country: United States

08-OCT-2001

Type: cooperating company
Name: R.T. Vanderbilt Company, Inc.
Country: United States

08-OCT-2001

Type: cooperating company
Name: The Goodyear Tire & Rubber Company
Country: United States

08-OCT-2001

Type: cooperating company
Name: The Lubrizol Corporation
Country: United States

08-OCT-2001

Type: cooperating company
Name: UOP, LLC.
Country: United States

08-OCT-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: > 95 % w/w
Remark: This substance is only supplied as an aqueous solutions (18-50%).
20-OCT-1999

1.1.0 Details on Template
-

1.1.1 Spectra
-

1.2 Synonyms

2(3H)-benzothiazolethione sodium salt
20-OCT-1999

2-mercaptobenzothiazole sodium salt
20-OCT-1999

SMBT
20-OCT-1999

Sodium MBT
20-OCT-1999

1.3 Impurities
-

1.4 Additives
-

1.5 Quantity
-

1.6.1 Labelling
-

1.6.2 Classification
-

1.7 Use Pattern

Type: type
Category: Non dispersive use
20-OCT-1999

Type: type
Category: Use resulting in inclusion into or onto matrix
20-OCT-1999

Type: industrial
Category: Chemical industry: used in synthesis
20-OCT-1999

Type: industrial
Category: Polymers industry
20-OCT-1999

Type: use
Category: Corrosive inhibitors
20-OCT-1999

Type: use
Category: Intermediates
20-OCT-1999

Type: use
Category: Vulcanizing agents
20-OCT-1999

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: 85.8 degree C
Method: other: MPBPWIN (v1.31)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Result: Melting Point: 155.34 deg C (Adapted Joback Method)
Melting Point: 62.56 deg C (Gold and Ogle Method)
Mean Melt Pt : 108.95 deg C (Joback; Gold,Ogle Methods)
Selected MP: 85.76 deg C (Weighted Value)
Accepted calculation method
Flag: Critical study for SIDS endpoint
08-OCT-2001 (1)

Value: = -6 degree C
Decomposition: no
Sublimation: no
Method: other: no data
GLP: no data
Testsubstance: other TS: 50% aqueous solution of sodium
Remark: Freezing point for an approximately 50% aqueous solution of sodium 2-mercaptobenzothiazole
Source: Monsanto Europe N.V. Bruxelles
08-OCT-2001 (2)

2.2 Boiling Point

Value: 301.8 degree C
Method: other: MPBPWIN (v1.31) Adapted Stein and Brown Method
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
08-OCT-2001 (1)

Value: = 103 degree C at 1013 hPa
Decomposition: no
Method: other: no data
GLP: no data
Testsubstance: other TS: 50% aqueous solution of sodium
Source: Monsanto Europe N.V. Bruxelles
08-OCT-2001 (2)

2.3 Density

Type: density
Value: = 1.25 g/cm3 at 25 degree C
GLP: no data
Source: Monsanto Europe N.V. Bruxelles
18-MAY-1994 (3)

Type: density
Value: ca. 1.3 g/cm3 at 25 degree C
Method: other: no data
GLP: no data
Source: Monsanto Europe N.V. Bruxelles
18-MAY-1994 (2)

2.3.1 Granulometry
-

2.4 Vapour Pressure

Value: .0006186 hPa at 25 degree C
Method: other (calculated): MPBPWIN (v1.31) Modified Grain Method
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Result: Vapor Pressure Estimations (25 deg C):
(Using BP: 301.80 deg C (estimated))
(Using MP: 85.76 deg C (estimated))
VP: 0.000356 mm Hg (Antoine Method)
VP: 0.000464 mm Hg (Modified Grain Method)
VP: 0.00084 mm Hg (Mackay Method)
Selected VP: 0.000464 mm Hg (Modified Grain Method)
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
08-OCT-2001 (1)

Value: = 32 hPa at 25 degree C
Method: other (measured): no data
GLP: no data
Testsubstance: other TS: 50% aqueous solution of sodium
Remark: Vapour pressure of sodium 2-mercaptobenzothizole would be expected to extremely low. The vapor pressure listed is due to the water present in the aqueous solution and not due to sodium 2-mercaptobenzothiazole.
Source: Monsanto Europe N.V. Bruxelles
08-OCT-2001 (4)

2.5 Partition Coefficient

log Pow: 2.86 at 25 degree C
Method: other (calculated): KOWWIN v1.65 Estimations Program
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Remark: Experimental database match = 2.42 (ref: TSCATS)
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
08-OCT-2001 (1)

log Pow: 2.42 at 25 degree C
Method:
Year:
Testsubstance: other TS: 2-Mercaptobenzothiazole
Reliability: (2) valid with restrictions
Data from Handbook or collection of data
Flag: Critical study for SIDS endpoint
08-OCT-2001 (5)

log Pow: = -.46
Method: other (measured)
Year: 1978
GLP: no data
Source: Monsanto Europe N.V. Bruxelles
Test condition: Method did not follow OECD guidelines. Samples analyzed at one concentration only.
26-APR-2001 (6)

2.6.1 Water Solubility

Value: 543.4 at 25 degree C
Method: other: WSKOW (v1.36)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Result: Log Kow (estimated) : 2.86
Log Kow (experimental): 2.42
Cas No: 000149-30-4
Name : 2-Mercaptobenzothiazole
Refer : TSCATS
Log Kow used by Water solubility estimates: 2.42

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW

Log Water Solubility (in moles/L) : -2.488
Water Solubility at 25 deg C (mg/L): 543.4
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
08-OCT-2001 (1)

Value: > 500 g/l at 25 degree C
pH: = 11.5 - 13.5 at 50 vol%
Method: other
GLP: no data
Source: Monsanto Europe N.V. Bruxelles
Flag: Critical study for SIDS endpoint
08-OCT-2001 (2)

2.6.2 Surface Tension
-

2.7 Flash Point

Value: > 93 degree C
Type: other
Method:
Year:
GLP: no data
Source: Monsanto Europe N.V. Bruxelles
18-MAY-1994 (2)

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: .0000000000406348 cm3/(molecule * sec)
Degradation: 50 % after 3.2 hour(s)
Method: other (calculated): AopWin v1.88
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
08-OCT-2001 (1)

3.1.2 Stability in Water

Type: abiotic
Method:
Year: GLP:
Test substance:
Remark: See IUCLID document on CAS# 140-30-4
09-OCT-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	0.507	6.32	1000	7.72e-012
Water	35.9	360	1000	4.06e-013
Soil	63.4	360	1000	2.76e-012
Sediment	0.172	1.44e+003	0	2.71e-013

Persistence Time: 347 hr
Reaction Time: 405 hr

Advection Time: 2.44e+003 hr
Percent Reacted: 85.8
Percent Advected: 14.2
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
08-OCT-2001 (1)

3.3.2 Distribution
-

3.4 Mode of Degradation in Actual Use
-

3.5 Biodegradation

Type: aerobic
Inoculum:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID document on CAS# 140-30-4
09-OCT-2001

3.6 BOD5, COD or BOD5/COD Ratio
-

3.7 Bioaccumulation

Species: other
Exposure period:
Concentration:
BCF: 14.57
Elimination:
Method: other: BCF Program (v2.13)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Result: Log Kow (estimated) : 2.86
Log Kow (experimental): 2.42
Log Kow used by BCF estimates: 2.42

Equation Used to Make BCF estimate:
Log BCF = 0.77 log Kow - 0.70

Estimated Log BCF = 1.163 (BCF = 14.57)
Reliability: (2) valid with restrictions
Accepted calculation method
08-OCT-2001 (1)

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: mg/l Analytical monitoring:
LC50: 12 - 15
Method: other: according to Northeastern Biologists (1976)
Year: 1976 GLP: no data
Test substance: other TS: NACAP, 50% aqueous sodium 2-mercaptobenzothiazole
Remark: The toxic effect took place during the first 24 hours of exposure.
Result:

Concentration (mg/l)	% mortality 24hrs	48hrs	72hrs	96hrs	Total
9.5	0	0	0	0	0
12.00	5	0	0	0	5
15.00	95	0	0	0	95
Control	0	0	0	5	5

Reliability: (1) valid without restriction
Meets generally accepted scientific method and is described in sufficient detail
Flag: Critical study for SIDS endpoint
08-OCT-2001 (7)

Type: static
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 2.58 - 3.16
Method: other: according to Northeastern Biologists (1976)
Year: GLP:
Test substance: other TS: NACAP, 50% aqueous sodium 2-mercaptobenzothiazole
Remark: The toxic effect took place during the first 24 hours of exposure.
Result:

Concentration (mg/l)	% mortality 24hrs	48hrs	72hrs	96hrs	Total
1.99	0	0	0	0	0
2.58	15	0	0	0	15
3.16	75	0	0	0	75
Control	0	0	0	0	0

Reliability: (1) valid without restriction
Meets generally accepted scientific method and is described in sufficient detail
Flag: Critical study for SIDS endpoint
08-OCT-2001 (7)

Type: other: calculation
Species: other
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: 7.254
Method: other: ECOSAR Program (v0.99e)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
08-OCT-2001 (1)

Type: static
Species: Lepomis macrochirus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: = 3.8
Method: other: Bionomics laboratory protocol; see test conditions
Year: 1976 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Remark: C.I.=3.2-4.4 mg/l; 24hr LC50=5.7 mg/l; 48hr LC50=4.5 mg/l
Source: Monsanto Europe N.V. Bruxelles
Test condition: carrier-acetone; 15 L dilution water; no food; length=3.8 cm; temp=22C
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
08-OCT-2001 (8)

Type: static
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: = 1.8
Method: other: Bionomics Laboratory protocol; see test conditions
Year: 1976 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Remark: C.I.=1.3-2.4 mg/l; 24hr LC50=2.0 mg/l; 48hr LC50=1.8 mg/l
Source: Monsanto Europe N.V. Bruxelles
Test condition: carrier-acetone; 15 L dilution water; length=3.7 cm; no food; temp=12C
08-OCT-2001 (8)

Type:
Species: Leuciscus idus (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no data
LC50: > 5
Method: other: test conditions undocumented
Year: 1985 GLP: no data
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles
08-OCT-2001 (9)

Type:
Species: Poecilia reticulata (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: Analytical monitoring:
Method: other
Year: GLP:
Test substance: other TS: UniRoyal NaMBT; purity not noted
Result: TLm = 12 ppm (48 hours) in tap water
08-OCT-2001 (10)

Type: other: calculation
Species: other
Exposure period: 14 day
Unit: mg/l Analytical monitoring: no
LC50: 40.021
Method: other: ECOSAR Program (v0.99e)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
08-OCT-2001 (1)

Type: static
Species: Oncorhynchus tschawytscha (Fish, fresh water, marine)
Exposure period: 4 hour(s)
Unit: mg/l Analytical monitoring: no
LC100: 10
Method: other: MacPhee, C. et al protocol; see test conditions
Year: 1969 GLP: no data
Test substance: no data
Remark: fish died after 2-4 hour exposure at 10 mg/l
Source: Monsanto Europe N.V. Bruxelles
Test condition: fish 5-10 cm long; acclimated; river water; temp=11C
08-OCT-2001 (11)

Type: static
Species: Ptychocheilus oregonensis (Fish, fresh water)
Exposure period: 11 hour(s)
Unit: mg/l Analytical monitoring: no data
LC100: 10
Method: other: MacPhee, C. et al protocol; see test conditions
Year: 1969 GLP: no data
Test substance: no data
Remark: fish died after 7-11 hour exposure at 10 mg/l
Source: Monsanto Europe N.V. Bruxelles
Test condition: fish 5-10 cm long; acclimated; river water; temp=11C
08-OCT-2001 (11)

4.2 Acute Toxicity to Aquatic Invertebrates

Type:
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
NOEC: = 10
EC50: = 19
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: 1984 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles
Test condition: carrier-acetone; temp=19C; well water; 16hr light
Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint
08-OCT-2001 (12)

Type: other: calculated
Species: Daphnia sp. (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 4.005
Method: other: ECOSAR Program (v0.99e)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
08-OCT-2001 (1)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Selenastrum capricornutum (Algae)
Endpoint: biomass
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: = .3
Method: OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year: 1984 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Remark: C.I.=.04-3 mg/l; in vivo chlorophyll EC50: 24hr=2 mg/l; 48hr=1 mg/l; 72hr=0.4 mg/l; 96hr=0.4 mg/l
Source: Monsanto Europe N.V. Bruxelles
Test condition: temp=24C; 4000 lux
Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint
08-OCT-2001 (13)

Species: other algae: green algae
Endpoint: growth rate
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 14.396
ChV : 2.367
Method: other: ECOSAR Program (v0.99e)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
08-OCT-2001 (1)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type:
Species: activated sludge
Exposure period: 3 hour(s)
Unit: mg/l Analytical monitoring: no data
EC50: = 857
Method: ISO 8192 "Test for inhibition of oxygen consumption by activated sludge"
Year: GLP: yes
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles
Reliability: (1) valid without restriction
GLP guideline study
08-OCT-2001 (14)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

Species: other
Endpoint: other
Exposure period: 30 day
Unit: mg/l Analytical monitoring: no
ChV : 1.084
Method: other: ECOSAR Program (v0.99e)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
08-OCT-2001 (1)

4.5.2 Chronic Toxicity to Aquatic Invertebrates

Species:	Daphnia sp. (Crustacea)	
Endpoint:	other	
Exposure period:	21 day	
Unit:	mg/l	Analytical monitoring: no
ChV :	c .784	
Method:	other: ECOSAR Program (v0.99e)	
Year:		GLP: no
Test substance:	other TS: molecular structure	
Reliability:	(2) valid with restrictions	
	Accepted calculation method	

08-OCT-2001 (1)

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:
Sex:
Number of Animals:
Vehicle:
Value: = 5200 mg/kg bw
Method: other: Younger Laboratory method
Year: 1978 GLP: no data
Test substance: other TS: 45% to 50% substance content
Source: Monsanto Europe N.V. Bruxelles
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
08-OCT-2001 (15)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 9500 mg/kg bw
Method: other: Younger Laboratory method
Year: 1987 GLP: yes
Test substance: other TS
Source: Monsanto Europe N.V. Bruxelles
Test substance: 22% substance content.
Reliability: (1) valid without restriction
GLP study, Meets generally accepted scientific method and is described in sufficient detail
Flag: Critical study for SIDS endpoint
08-OCT-2001 (16)

Type: LD50
Species: rat
Strain:
Sex: male
Number of Animals:
Vehicle:
Value: = 750 mg/kg bw
Method: other: Acute Oral Toxicity
Year: 1965 GLP: no data
Test substance: other TS
Result:

Dose (ml/kg)	mortality
0.625	1/5

1.25	2/5
2.5	3/5
5.0	5/5

Signs of intoxication: tremors, convulsion, severe depression and hematuria.

Gross autopsy findings: decedents - hemorrhage of stomach
survivors - normal

Source: Monsanto Europe N.V. Bruxelles
Test substance: 50% Na-2-mercaptobenzothiazole solution
08-OCT-2001 (17)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 4350 mg/kg bw
Method: other
Year: 1974 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles
Test substance: Unknown sulfur content.
27-MAY-1994 (18)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 2160 mg/kg bw
Method: other: Acute Oral Toxicity
Year: 1973 GLP: no data
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles
23-MAY-1994 (19)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 3968 mg/kg bw
Method: other: Acute Oral Toxicity
Year: 1975 GLP: no data
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles
23-MAY-1994 (20)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 3120 mg/kg bw
Method: other: Acute Oral Toxicity
Year: 1980 GLP: no data
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles
23-MAY-1994 (21)

Type: LD100
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 2500 mg/kg bw
Method: other: Acute Oral Toxicity
Year: 1975 GLP: no data
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles
23-MAY-1994 (22)

Type: LD100
Species: rat
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: = 3125 mg/kg bw
Method: other: Acute Oral Toxicity
Year: 1965 GLP: no data
Test substance: other TS
Remark: male rats only
Source: Monsanto Europe N.V. Bruxelles
Test substance: 50% Na-2-mercaptobenzothiazole
03-JUN-1994 (17)

Type: other
Species: rat
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: > 625 mg/kg bw
Method: other: Acute Oral Toxicity
Year: 1975 GLP: no data
Test substance: no data
Remark: male rat mortality:

1) 312.5 mg/kg bw - 1/5
2) 625 mg/kg bw - 2/5
3) 1250 mg/kg bw - 3/5

Source: Monsanto Europe N.V. Bruxelles
23-MAY-1994 (23)

Type: other
Species: rat
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: > 391 mg/kg bw
Method: other: Acute Oral Toxicity
Year: 1965 GLP: no data
Test substance: other TS
Remark: male rat mortality:

1) 391 mg/kg bw, 1/5
2) 782 mg/kg bw, 2/5
3) 1563 mg/kg bw, 3/5

Source: Monsanto Europe N.V. Bruxelles
Test substance: 50% Na-2-mercaptobenzothiazole
03-JUN-1994 (17)

Type: other
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: > 2000 mg/kg bw
Method: other: Acute Oral Toxicity
Year: 1963 GLP: no data
Test substance: no data
Remark: mortality:

1) 2000 mg/kg bw, 0/2
2) 3980 mg/kg bw, 3/3
Source: Monsanto Europe N.V. Bruxelles
23-MAY-1994 (24)

Type: LD50
Species: mouse
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 1792 mg/kg bw
Method: other: Acute Oral Toxicity
Year: 1948 GLP: no data
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles
23-MAY-1994 (25)

Type: LD0
Species: mouse
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 708 mg/kg bw
Method: other: Acute Oral Toxicity
Year: 1948 GLP: no data
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles
23-MAY-1994 (26)

Type: LD100
Species: mouse
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 2560 mg/kg bw
Method: other: Acute Oral Toxicity
Year: 1948 GLP: no data
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles
23-MAY-1994 (25)

5.1.2 Acute Inhalation Toxicity

Type: LC50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Exposure time: 6 hour(s)
Value: > 8.2 mg/l
Method: other: Younger Laboratory method
Year: 1987 GLP: yes
Test substance: other TS
Source: Monsanto Europe N.V. Bruxelles
Test substance: 22% substance content.
Reliability: (1) valid without restriction
GLP study, Meets generally accepted scientific method and is described in sufficient detail
Flag: Critical study for SIDS endpoint
08-OCT-2001 (16)

Type: LC50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Exposure time: 6 hour(s)
Value: > 6.5 mg/l
Method: other: Younger Laboratory method
Year: 1978 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
08-OCT-2001 (27)

Type: LC50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Exposure time: 7 hour(s)
Value:
Method: other: Acute Inhalation Toxicity
Year: 1963 GLP: no data
Test substance: no data
Remark: Exposure to a saturated atmosphere resulted in 0/4 mortality
Source: Monsanto Europe N.V. Bruxelles
08-OCT-2001 (28)

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rabbit
Strain:
Sex:
Number of Animals:
Vehicle:
Value: > 5010 mg/kg bw
Method: other: Younger Laboratory method
Year: 1978 GLP: no data
Test substance: other TS: 45% to 50% substance content
Source: Monsanto Europe N.V. Bruxelles
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
08-OCT-2001 (15)

Type: LD50
Species: rabbit
Strain:
Sex:
Number of Animals:
Vehicle:
Value: > 7940 mg/kg bw
Method: other: Younger Laboratory method
Year: 1987 GLP: yes
Test substance: other TS: 22% substance content.
Source: Monsanto Europe N.V. Bruxelles
Reliability: (1) valid without restriction
GLP study, Meets generally accepted scientific method and is described in sufficient detail
Flag: Critical study for SIDS endpoint
08-OCT-2001 (16)

Type: LD50
Species: rabbit
Strain:
Sex:
Number of Animals:
Vehicle:
Value: > 3125 mg/kg bw
Method: other: Acute Dermal Toxicity
Year: 1965 GLP: no data
Test substance: other TS
Remark: male rabbit mortality:

1) 782 mg/kg bw, 0/10
2) 1563 mg/kg bw, 1/10
3) 3125 mg/kg bw, 4/10

Source: Monsanto Europe N.V. Bruxelles
Test substance: 50% Na-2-mercaptobenzothiazole
08-OCT-2001 (29)

Type: LD50
Species: rabbit
Strain:
Sex:
Number of Animals:
Vehicle:
Value: > 1250 mg/kg bw
Method: other: Acute Dermal Toxicity
Year: 1975 GLP: no data
Test substance: other TS
Remark:

Dose (ml/kg)	Dose (mg/kg bw)	mortality
1.25	313	0/10
2.5	625	1/10
5.0	1250	4/10

Signs of intoxication: severe depression, cold extremities, appetite loss.

Skin irritation: severe degree of skin injury. Area burned at 24 hours with formation of hard eschar at 1-2 weeks.

Gross autopsy findings: normal
Source: Monsanto Europe N.V. Bruxelles
Test substance: 50% Na-2-mercaptobenzothiazole
08-OCT-2001 (30)

Type: LD50
Species: rabbit
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: > 7940 mg/kg bw
Method: other: Younger Laboratory method
Year: 1974 GLP: no data
Test substance: other TS
Source: Monsanto Europe N.V. Bruxelles
Test substance: Unknown substance content.
08-OCT-2001 (18)

5.1.4 Acute Toxicity, other Routes
-

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result: corrosive
EC classificat.:
Method: other: Younger Laboratory method
Year: 1978 GLP: no data
Test substance: other TS
Remark: Use of 24-hour exposure data prohibits direct classification.
Source: Monsanto Europe N.V. Bruxelles
Test substance: 45% to 50% substance content.
03-JUN-1994 (15)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result: corrosive
EC classificat.: corrosive (causes burns)
Method: other: Younger Laboratory method
Year: 1978 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles
Test substance: 45% to 50% substance content.
03-JUN-1994 (31)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result: moderately irritating
EC classificat.:
Method: other: Younger Laboratory method
Year: 1987 GLP: yes
Test substance: other TS
Remark: Use of 24-hour exposure data prohibits direct classification.
Source: Monsanto Europe N.V. Bruxelles
Test substance: 22% substance content.
01-JUN-1994 (16)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result: highly irritating
EC classificat.:
Method: other: Younger Laboratory method
Year: 1974 GLP: no data
Test substance: other TS
Remark: Use of 24-hour exposure data prohibits direct classification.
Source: Monsanto Europe N.V. Bruxelles
Test substance: Unknown substance content.
03-JUN-1994 (18)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result: highly corrosive
EC classificat.:
Method: other: Skin Irritation
Year: 1975 GLP: no data
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles
27-MAY-1994 (23)

Species: human
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result: slightly irritating
EC classificat.:
Method: other: Skin Irritation
Year: 1962 GLP: no data
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles
27-MAY-1994 (32)

5.2.2 Eye Irritation

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of
Animals:
Result: corrosive
EC classificat.: risk of serious damage to eyes
Method: other: Younger Laboratory method
Year: 1978 GLP: no data
Test substance: other TS
Source: Monsanto Europe N.V. Bruxelles
Test substance: 45% to 50% sodium MBT content.
03-JUN-1994 (15)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: moderately irritating
EC classificat.: irritating
Method: other: Younger Laboratory method
Year: 1987 GLP: yes
Test substance: other TS
Source: Monsanto Europe N.V. Bruxelles
Test substance: 22% substance content.
01-JUN-1994 (16)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: moderately irritating
EC classificat.: irritating
Method: other: Younger Laboratory method
Year: 1974 GLP: no data
Test substance: other TS
Source: Monsanto Europe N.V. Bruxelles
Test substance: Unknown substance content.
03-JUN-1994 (33)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: corrosive
EC classificat.: risk of serious damage to eyes
Method: other: Acute Eye Irritation
Year: 1975 GLP: no data
Test substance: no data
Source: Monsanto Europe N.V. Bruxelles
23-MAY-1994 (23)

5.3 Sensitization
-

5.4 Repeated Dose Toxicity

Species: Sex:
Strain:
Route of admin.:
Exposure period:
Frequency of treatment:
Post. obs. period:
Doses:
Control Group:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID document on CAS# 140-30-4
09-OCT-2001

5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538
Concentration: up to 4.73 mg/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: Plate Incorporation Assay
Year: 1976 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles
Reliability: (2) valid with restrictions
22% substance content.
Flag: Critical study for SIDS endpoint
08-OCT-2001 (34)

Type: Mammalian cell gene mutation assay
System of testing: Balb/3T3 cells
Concentration: 78.0 to 13.0 nl/ml
Cytotoxic Conc.:
Metabolic activation:
Result: negative
Method: Directive 87/302/EEC, part B, p. 73 "Mutagenicity: - In vitro mammalian cell transformation tests"
Year: 1982 GLP:
Test substance: other TS: NACAP; purity not noted
Result: The test substance did not induce the appearance of a significant number of transformed foci over the concentration range of 78.0 to 13.0 nl/ml. Therefore the test substance is considered to be inactive in the Balb/3T3 in vitro Transformation Assay.

Source: Goodyear Tire & Rubber Company
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
08-OCT-2001 (35)

Type: Yeast gene mutation assay
System of testing: Saccharomyces cerevisiae D4
Concentration: up to 4.73 mg/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: Plate Incorporation Assay
Year: 1976 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Source: Monsanto Europe N.V. Bruxelles
08-OCT-2001 (36)

Type: Ames test
System of testing: Salmonella typhimurium
Concentration:
Cytotoxic Conc.:
Metabolic activation:
Result: ambiguous
Method: other
Year: 1983 GLP: no data
Test substance: no data
Remark: weakly positive, no other data available
Source: Monsanto Europe N.V. Bruxelles
08-OCT-2001 (37)

5.6 Genetic Toxicity 'in Vivo'

Type:
Species: Sex:
Strain:
Route of admin.:
Exposure period:
Doses:
Result:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID document on CAS# 140-30-4
09-OCT-2001

5.7 Carcinogenicity

Species: Sex:
Strain:
Route of admin.:
Exposure period:
Frequency of
treatment:
Post. obs.
period:
Doses:
Result:
Control Group:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID document on CAS# 140-30-4 and #155-04-4
09-OCT-2001

5.8 Toxicity to Reproduction

Type:
Species: Sex:
Strain:
Route of admin.:
Exposure Period:
Frequency of
treatment:
Duration of test:
Doses:
Control Group:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID document on CAS# 140-30-4
09-OCT-2001

5.9 Developmental Toxicity/Teratogenicity

Species: Sex:
Strain:
Route of admin.:
Exposure period:
Frequency of
treatment:
Duration of test:
Doses:
Control Group:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID document on CAS# 140-30-4
09-OCT-2001

5.10 Other Relevant Information
-

5.11 Experience with Human Exposure
-

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

(2) Monsanto manufacturing data.

(3) ITC/USEPA; Information review #351 p. 2 1983.

(4) Monsanto manufacturing data for 50% aqueous solution.

(5) TSCATS

(6) Monsanto study ES-78-SS20.

(7) R.T. Vanderbilt Study by Northeastern Biologists, Inc. 2-3-1976

(8) Monsanto report BN-76-0168

(9) Syracuse Research Corporation (1985), Technical Support Document 2-Mercaptobenzothiazoles, Final Draft

(10) Uniroyal Ltd. Short report, August 12, 1982

(11) MacPhee, C. and R. Ruelle (1969), Lethal effects of 1888 chemicals upon four species of fish from western North America, Forest, Wildlife and Range Exp. Stat. Bulletin No. 3.

(12) Monsanto report AB-78-0357

Syracuse Research Corporation (1985), Technical Support Document 2-Mercaptobenzothiazoles, Final Draft

(13) Monsanto report BN-78-0359

(14) Bayer AG report

(15) Monsanto report YO-78-0122.

(16) Monsanto report YO-87-0227.

(17) American Cyanamid Co. (1965). Toxicity data on sodium MBT solution. Report No. 65-1. Cited in: Technical Support Document, Contract No. 68-02-4209, task 6, Syracuse Research Corporation (1985)

(18) Monsanto report YO-74-0019.

(19) Toxic Substances Technical Data Sheet. Vanderbilt Co., R.T. New York (1973): cited in: Toxicity Summary WTR. No. 23a

(20) R.T. Vanderbilt Co. (1975). Material Safety Data Sheet - Sodium 2-Mercaptobenzothiazole, Norwalk, CT. Cited in: Syracuse Research Corporation (1976): NTIS/PB 256662

(21) Farm Chemicals Handbook. (1980). Cited in: RTECS (1988).

(22) American Cyanamid Co. (1975). Personal communication, Wayne, New Jersey. Cited in: Syracuse Research Corporation (1976) - NTIS/PB 256662

(23) American Cyanamid Co. (1975). Personal Communication, Wayne, New Jersey. Cited in: Syracuse Research Corporation (1976) - NTIS/PB 256662

(24) Dow Chemical Co. (1985). TSCA Sec. 8(d) submission 878214939. Cited in: Technical Support Document, Contract No. 68-02-4209, task 6, Syracuse Research Corporation (1985)

(25) Goodyear. (1948). Munich Research Lab Report No. 48164. Cited in: Toxicity Summary WTR No. 23a

(26) Goodyear. (1948). Munich Research Lab Report No. 48164. Cited in: Toxicity Summary WTR 23a

(27) Monsanto report YO-78--122.

(28) Dow Chemical Co. (1985). TSCA Section 8(d) submission 878214939. Cited in: Technical Support Document, Contract No. 68-02-4209, task 6, Syracuse Research Corporation (1985)

(29) American Cyanamid Co. (1965). Toxicity data on sodium MBT Solution. Report No. 65-1. Cited in: Technical Support Document, Contact No. 68-02-4209, task 6, Syracuse Research Corporation (1985)

(30) American Cyanamid Co. (1975). Personal Communication, Wayne, New Jersey. Cited in: Syracuse Research Coprporation (1976) - NTIS/PB 256662

(31) Monsanto report YO-78-0283.

(32) Fregert, S. and E. Skog. (1962). Acta Dermato-Venereologica 42, 235-238

(33) Monsanto report Y-74-0019.

(34) Litton Bionetics Inc. (1976). LBI Project No. 2683.

(35) Litton Bionetics LBI #20992

(36) Litton Bionetics Inc. (1976). LBI Project No. 2683

(37) NTP. (1984). Annual plan for fiscal year 1984, NTP-84-023

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: 95-16-9
CAS No.	95-16-9
EINECS Name	benzothiazole
EINECS No.	202-396-2
Molecular Weight	135.2
Molecular Formula	C7H5NS

Producer Related Part	
Company:	
Creation date:	08-JUL-1994
Substance Related Part	
Company:	
Creation date:	08-JUL-1994
Memo:	Data for RAPA Benzothiazole-based Thiazoles category
Printing date:	09-OCT-2001
Revision date:	
Date of last Update:	30-MAY-1995
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
-

1.0.2 Location of Production Site
-

1.0.3 Identity of Recipients
-

1.1 General Substance Information

Substance type: organic
Physical status: liquid
08-JUL-1994

1.1.0 Details on Template
-

1.1.1 Spectra
-

1.2 Synonyms

Benzothiazol
08-JUL-1994

1.3 Impurities
-

1.4 Additives
-

1.5 Quantity
-

1.6.1 Labelling

-

1.6.2 Classification

-

1.7 Use Pattern

Type: type
Category: Non dispersive use
30-MAY-1995

Type: type
Category: Use in closed system
08-JUL-1994

Type: industrial
Category: Chemical industry: used in synthesis
08-JUL-1994

Type: use
Category: Intermediates
08-JUL-1994

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: ca. 2 degree C
08-JUL-1994 (1)

2.2 Boiling Point

Value: ca. 230 degree C
08-JUL-1994 (1)

2.3 Density

Type: density
Value: ca. 1.246 at 20 degree C
08-JUL-1994 (1)

2.3.1 Granulometry
-

2.4 Vapour Pressure

Value: ca. .13 hPa at 20 degree C
30-MAY-1995 (1)

Value: ca. .95 hPa at 50 degree C
30-MAY-1995 (1)

2.5 Partition Coefficient

log Pow: 2
Method: other (calculated): Leo, Hansch: Leo, A. CLOGP-3.63 (1991) Daylight, Chemical Information Systems Inc. Irvine, CA, USA
Year:
30-MAY-1995 (2)

log Pow: 2.01
Method: other (measured)
Year:
08-JUL-1994 (3)

2.6.1 Water Solubility

Value: ca. 3 g/l at 20 degree C
08-JUL-1994 (1)

2.6.2 Surface Tension
-

2.7 Flash Point

Value: ca. 107 degree C
Type:
Method: other: DIN 51758
Year:
08-JUL-1994 (1)

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
Method: other (calculated): acc. to Atkinson: SRC-AOP for Microsoft Windows
Year: GLP:
Test substance:
Remark: Sensitizer: OH
Conc. of Sensitizer: 0.5E6 OH/cm3
Rate Constant: 7.0E-12 cm3/molecule x sec
Half life time: 4.584 d
05-MAY-1995 (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
-

3.3.2 Distribution
-

3.4 Mode of Degradation in Actual Use
-

3.5 Biodegradation

Type: aerobic
Inoculum: predominantly domestic sewage
Concentration: .8 mg/l
Degradation: > 65 % after 21 day
Method: OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
Year: 1984 GLP: no
Test substance:
11-AUG-1994 (5)

Type: aerobic
Inoculum: other: sludge samplings from different sewage plants, rivers, bays and a lake
Concentration: 100 mg/l related to Test substance
Degradation: 0 % after 28 day
Method: other: see remarks
Year: GLP: no data
Test substance:
Remark: related to BOD
sludge conc.: 30 mg/l
Method:
"Biodegradation test of chemical substance by microorganisms etc." stipulated in the Order Prescribing the Items of the Test Relating to the New Chemical Substance (1974, Order of the Prime Minister, Minister of Health and Welfare, the MITI No. 1). This guideline corresponds to "301C, Ready Biodegradability: Modified MITI Test I" stipulated in the OECD Guidelines for Testing of Chemicals (May 12, 1981).
17-AUG-1994 (6)

3.6 BOD5, COD or BOD5/COD Ratio

Remark: ThOD: 2553 mg/g
COD: 2157 mg/g
11-AUG-1994 (5)

3.7 Bioaccumulation

Species: Cyprinus carpio (Fish, fresh water)
Exposure period: 42 day
Concentration:
BCF:
Elimination:
Method:
Year: GLP: no data
Test substance:
Remark:

Conc. (mg/l)	BCF
0.2	2.1-5.1
0.02	< 4.1-7.5

% lipid, average 4.0
Method:
"Bioaccumulation test of chemical substance in fish and shellfish" stipulated in the Order Prescribing the Items of the Test Relating to the New Chemical Substance (1974, Order of the Prime Minister, the Minister of Health and Welfare, the MITI No. 1). This guideline corresponds to "305C, Bioaccumulation: Degree of Bioconcentration in Fish" stipulated in the OEDC Guidelines for Testing of Chemicals (May 12, 1981).
11-AUG-1994 (6)

3.8 Additional Remarks
-

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: flow through
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: yes
LC50: 64
Method:
Year: 1989 GLP:
Test substance: other TS: > 96 %
Remark: 96h-EC50: 60.7 mg/l
Analtyical monitoring: GLC
17-OCT-1994 (7)

Type: static
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC0: 65.5
LC100: 66
Method: other: DIN 38 412, Teil 15: Bestimmung der Wirkung von Wasserinhaltsstoffen auf Fische, Fischtest (L 15) (Juni 1982)
Year: 1984 GLP: no
Test substance:
11-AUG-1994 (5)

Type:
Species: Oryzias latipes (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 87.2
Method: other: Japanese Industrial Standard (JIS K 0102-1986-71) "Testing methods for industrial waste water"
Year: GLP: no data
Test substance:
11-AUG-1994 (6)

Type:
Species: Oryzias latipes (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 110
Method:
Year: GLP: no
Test substance:
Remark: QSAR calculation
17-AUG-1994 (8)

4.2 Acute Toxicity to Aquatic Invertebrates
-

4.3 Toxicity to Aquatic Plants e.g. Algae
-

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: 635
EC05 : 216
Method: ISO 8192 "Test for inhibition of oxygen consumption by activated sludge"
Year: 1990 GLP: no
Test substance:
11-AUG-1994 (5)

Type: aquatic
Species: Pseudomonas putida (Bacteria)
Exposure period: 30 minute(s)
Unit: mg/l Analytical monitoring: no
LC0 : 250
Method: other: Bewetung 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: 1984 GLP: no
Test substance:
11-AUG-1994 (5)

Type: aquatic
Species: Pseudomonas putida (Bacteria)
Exposure period: 18 hour(s)
Unit: mg/l Analytical monitoring: no
LC0 : 50
Method:
Year: 1990 GLP: no
Test substance:
Remark: Method:
Grenzwerte der Schadwirkung wassergefaehrdender Stoffe gegen Bakterien (Pseudomonas putida) und Gruenalgen (Scenedesmus quadricauda) im Zellvermehrungshemmtest. Bringmann, G.; Kuehn, R.: Z. f. Wasser- und Abwasser-Forschung 10 (3/4), 87-98 (1977)
07-OCT-1994 (5)

Type: aquatic
Species: Tetrahymena pyriformis (Protozoa)
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring: no data
EC50: 160
Method: other: static at 30 degrees C
Year: GLP: no data
Test substance: other TS: analytical grade
07-OCT-1994 (9)

Type:
Species: activated sludge
Exposure period: 3 hour(s)
Unit: mg/l Analytical monitoring:
EC50: 650
Method: OECD Guide-line 209 "Activated Sludge, Respiration Inhibition Test"
Year: GLP:
Test substance:
17-AUG-1994 (8)

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:			
Sex:			
Number of Animals:			
Vehicle:			
Value:	= 479 mg/kg bw		
Method:	other		
Year:	1986	GLP: yes	
Test substance:	other TS		
Remark:	value = 493.3 mg/kg (m), 465.6 mg/kg (f)		
Test substance:	purity: 99 %		
27-JUL-1994			(10)

Type:	LD50		
Species:	rat		
Strain:			
Sex:			
Number of Animals:			
Vehicle:			
Value:	= 257 mg/kg bw		
Method:	other		
Year:	1982	GLP: no	
Test substance:	no data		
Remark:	value = 0.206 ml/kg; density: 1.246 g/l; male rat		
27-JUL-1994			(11)

Type:	LD50		
Species:	rat		
Strain:			
Sex:			
Number of Animals:			
Vehicle:			
Value:	= 177 mg/kg bw		
Method:	other		
Year:	1982	GLP: no	
Test substance:	no data		
Remark:	value = 0.142 ml/kg; density: 1.246 g/l; female rat		
27-JUL-1994			(12)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value:
Method: other
Year: GLP: no data
Test substance: no data
Remark: dependent on the number of animals in each dose group LD50 values from 180 (1 rat/dose) to 375 mg/kg (5 rats/dose) were calculated
27-JUL-1994 (13)

Type: LD50
Species: mouse
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 900 mg/kg bw
Method: other
Year: GLP: no data
Test substance: no data
27-JUL-1994 (14)

Type: other
Species: cat
Strain:
Sex:
Number of Animals:
Vehicle:
Value:
Method: other
Year: 1985 GLP: no
Test substance: other TS
Remark: 2 cats, 25 mg/kg with gavage: slightly elevated MetHb concentration (up to ca. 10 % after 3 hours), no effect after 7 hours; up to 100 % of the erythrocytes with Heinz bodies
Test substance: purity: ca. 98 %
27-JUL-1994 (15)

5.1.2 Acute Inhalation Toxicity

Type:	LC50
Species:	rat
Strain:	
Sex:	
Number of Animals:	
Vehicle:	
Exposure time:	4 hour(s)
Value:	ca. 5 mg/l
Method:	OECD Guide-line 403 "Acute Inhalation Toxicity"
Year:	1992 GLP: yes
Test substance:	other TS
Remark:	the following analytical concentrations were tested: 0.377 mg/l (vapour); 2.36 mg/l (aerosol) and 6.154 mg/l (aerosol) (analytical aerosol concentration)
Test substance:	purity: 97.4 %

27-JUL-1994 (16)

Type:	other: LC
Species:	rat
Strain:	
Sex:	
Number of Animals:	
Vehicle:	
Exposure time:	6 hour(s)
Value:	> 1.5 mg/l
Method:	other: no data
Year:	GLP: no data
Test substance:	no data

27-JUL-1994 (17)

5.1.3 Acute Dermal Toxicity

Type:	LD50
Species:	rat
Strain:	
Sex:	
Number of Animals:	
Vehicle:	
Value:	
Method:	other: Directive 84/449EEC, B.3.
Year:	1992 GLP: yes
Test substance:	other TS
Remark:	value: 1231 mg/kg (m), 933 mg/kg (f) NOEL = 500 mg/kg
Test substance:	purity: 97.4 %

27-JUL-1994 (18)

Type: LD50
Species: rabbit
Strain:
Sex:
Number of Animals:
Vehicle:
Value: > 631 mg/kg bw
Method: other: no data
Year: GLP: no data
Test substance: no data
27-JUL-1994 (17)

5.1.4 Acute Toxicity, other Routes

Type: LD50
Species: mouse
Strain:
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.p.
Value: ca. 100 - 200 mg/kg bw
Method: other: no data
Year: GLP: no data
Test substance: no data
28-JUL-1994 (19)

Type: LD50
Species: mouse
Strain:
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.v.
Value: = 95 mg/kg bw
Method: other: no data
Year: GLP: no data
Test substance: no data
28-JUL-1994 (20)

Type: LDLo
Species: other
Strain:
Sex:
Number of
Animals:
Vehicle:
Route of admin.: other
Value:
Method: other: no data
Year: GLP: no data
Test substance: no data
Remark: cat, i.v. 100 mg/kg; rat, i.v. 200-300 mg/kg;
rat, i.p. 1000 mg/kg; rat, oral 3000 mg/kg
27-JUL-1994 (21)

Type: LD50
Species: mouse
Strain:
Sex:
Number of
Animals:
Vehicle:
Route of admin.: other: no data
Value: = 310 mg/kg bw
Method: other: no data
Year: GLP: no data
Test substance: no data
27-JUL-1994 (22)

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: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year: 1983 GLP: no
Test substance: no data
27-JUL-1994 (23)

5.2.2 Eye Irritation

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: irritating
EC classificat.:
Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year: 1983 GLP: no
Test substance: no data
27-JUL-1994 (24)

5.3 Sensitization
-

5.4 Repeated Dose Toxicity
-

5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: S. typhimurium TA 98, TA 100, TA 1535, TA 1537
Concentration: up to 5000 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: see remark
Year: 1991 GLP: yes
Test substance: other TS
Remark: method: as described by Ames, B.N. et al., Proc. nat. Acad. Sci. (USA) 70, 2281-2285 (1973); Ames, B.N. et al., Mutat. Res. 31, 347-364 (1975) and Maron, D.M. & Ames, B.N., Mutat. Res. 113, 173-215 (1983)
Test substance: purity: 97.4 %
27-JUL-1994 (25)

5.6 Genetic Toxicity 'in Vivo'
-

5.7 Carcinogenicity
-

5.8 Toxicity to Reproduction
-

5.9 Developmental Toxicity/Teratogenicity
-

5.10 Other Relevant Information

Type: other
Remark: generation of chapter 5: July, 1994
27-JUL-1994

Type: other: Paralyzing potency
Remark: mouse, i.v.: median paralyzing dose (PD50) = 68 mg/kg
Test substance: no data
28-JUL-1994 (20)

5.11 Experience with Human Exposure

Remark: Upon the flexor surface of the left wrist of 43 subjects (5f/38m) approx. 25 mg/kg were placed; 17 subjects with positive reactions (no further information)
Test substance: other TS
27-JUL-1994 (21)

(1) Safety Data Sheet Bayer AG

(2) Calculation Bayer AG, WV-UWS

(3) THOR database Pomona 89, MedChemSoftware 1989, Daylight, Chemical Information Systems, Claremont, CA 91711, USA

(4) Calculation Bayer AG, WV-UWS/Produktsicherheit 1995

(5) Bayer AG data

(6) Biodegradation and Bioaccumulation Data of Existing Chemicals Based on the CSCL Japan, Compiled under the Supervision of Chemical Products Safety Division, Basic Industries Bureau MITI, Ed. by CITI, October 1992. Published by Japan Chemical Industry Ecology-Toxicology & Information Center

(7) Geiger, D.L. et al., Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales promelas) Vol. V, Center for Lake Superior Environmental Studies, University of Wisconsin-Superior, WI, ISBN 0-9614968-5-1 (1990)

(8) Yoshioka, Y. et al., Ecotox. Environ. Saf. 12 (3), 206-212 (1986)

(9) Yoshioka, Y. et al., The Science of the Total Environment 43, 149-157 (1985)

(10) Mayhew, D.A. et al., American Biogenics Corporation, AD-A172-647 September 1986

(11) Loeser, E., Untersuchungen zur akuten oralen Toxizitaet an maennlichen Ratten, July 27, 1982

(12) Loeser, E., Untersuchungen zur akuten oralen Toxizitaet an weiblichen Ratten, July 29, 1982

(13) Lorke, D., Arch. Toxicol. 54, 275-287 (1983)

(14) Moran, E.J. & Easterday, O.D., Drug Chem. Toxicol. 3, 249-258 (1980)

(15) Schmidt, W.M. & Loeser, E., Untersuchungen zur akuten oralen Toxizitaet an der Katze, December 20, 1985

(16) Bayer AG data, Report No. 21675, September 16, 1992

(17) United States EPA, Office of Pesticides and Toxic Substances. 8EHQ-1190-0987S, cited in RTECS April 1994

(18) Bayer AG data, Report No. 20998, January 21, 1992

(19) Doull, J. et al., AD277-689, 1-124 (1962)

(20) Domino, E.F. et al., J. Pharm. Exp. Ther. 105, 486-497 (1952)

(21) Bogert, M.T. & Husted, H.G., J. Pharm. Exp. Ther. 45, 189-207 (1932)

(22) Anonymous, Khimiko Farmatsevticheskii Zhurnal 9 (12), 11 (1975), cited in RTECS April 1994

(23) Suberg, H., Untersuchungen auf primaere Reiz-/Aetzwirkung an der Kaninchenhaut, January 3, 1983

(24) Suberg, H., Untersuchungen auf Schleimhautreizwirkung am Kaninchenauge, January 3, 1983

(25) Bayer AG data, Report No. 20847, November 26, 1991

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

New Chemical	ID: 95-32-9
CAS No.	95-32-9
EINECS Name	benzothiazole, 2-(4-morpholinyldithio)-
EINECS No.	202-410-7
Molecular Formula	C11H12N2OS3
Molecular Weight	284.42
Structural Formula	c1ccc2)c2)s1)C3)C3

Producer Related Part
Company:
Creation date: 29-SEP-2000

Substance Related Part
Company:
Creation date: 29-SEP-2000

Memo: Rubber and Plastics Additives (RAPA) HPV Panel

Printing date: 09-OCT-2001
Revision date:
Date of last Update: 09-OCT-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: American Chemistry Council (formerly Chemical Manufacturers Association) Rubber and Plastic Additives (RAPA) HPV Panel
Street: 1300 Wilson Boulevard
Town: 22209 Arlington, VA
Country: United States
Phone: 703-741-5600

28-SEP-2001

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

28-SEP-2001

Type: cooperating company
Name: Ciba Specialty Chemicals Corporation
Country: United States

28-SEP-2001

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

28-SEP-2001

Type: cooperating company
Name: Flexsys America L.P.
Country: United States

28-SEP-2001

Type: cooperating company
Name: Noveon, Inc
Country: United States

28-SEP-2001

Type: cooperating company
Name: R.T. Vanderbilt Company, Inc.
Country: United States

28-SEP-2001

Type: cooperating company
Name: The Goodyear Tire & Rubber Company
Country: United States

28-SEP-2001

Type: cooperating company
Name: The Lubrizol Corporation
Country: United States

28-SEP-2001

Type: cooperating company
Name: UOP, LLC.
Country: United States

28-SEP-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: 95 % w/w
Source: BFGoodrich Company
18-APR-2001

1.1.0 Details on Template
-

1.1.1 Spectra
-

1.2 Synonyms

2-(morpholinodithio)benzoliazole
18-APR-2001

2-benzothiazoyl morpholino disulfide
18-APR-2001

4-morpholinyl-2-benzothiazyl disulfide
18-APR-2001

Accelerator MF
18-APR-2001

Cure-Rite MBDS
18-APR-2001

Morfax
18-APR-2001

morpholino-2-benzothiazolyl disulfide
18-APR-2001

N-morpholinyl-2-benzothiazolyl disulfide
18-APR-2001

N-oxydiethyl-2-benzthiazolsulfenamid
18-APR-2001

Sulfenex MOB
18-APR-2001

Vulcuran 2
18-APR-2001

1.3 Impurities

CAS-No: 102-77-2
EINECS-No: 203-052-4
EINECS-Name: 2-(morpholinothio)benzothiazole
Contents: 1 % w/w
Source: BFGoodrich Company
18-APR-2001

CAS-No: 120-78-5
EINECS-No: 204-424-9
EINECS-Name: di(benzothiazol-2-yl) disulphide
Contents: .1 % w/w
Source: BFGoodrich Company
18-APR-2001

1.4 Additives

CAS-No: 8042-47-5
EINECS-No: 232-455-8
EINECS-Name: White mineral oil (petroleum)
Contents: 2 % w/w
18-APR-2001

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:	173.1 degree C
Method:	other: MPBPWIN (v1.31)
Year:	1999
GLP:	no
Testsubstance:	other TS: molecular structure
Result:	Melting Point: 343.10 deg C (Adapted Joback Method) Melting Point: 130.59 deg C (Gold and Ogle Method) Mean Melt Pt : 236.85 deg C (Joback; Gold,Ogle Methods) Selected MP: 173.09 deg C (Weighted Value)
Reliability:	(2) valid with restrictions Accepted calculation method
Flag:	Critical study for SIDS endpoint

28-SEP-2001 (1)

2.2 Boiling Point

Value:	418.3 degree C
Method:	other: MPBPWIN v1.31 (Adapted Stein and Brown Method)
Year:	1999
GLP:	no
Testsubstance:	other TS: molecular structure
Reliability:	(2) valid with restrictions Accepted calculation method
Flag:	Critical study for SIDS endpoint

28-SEP-2001 (1)

2.3 Density
-

2.3.1 Granulometry
-

2.4 Vapour Pressure

Value:	.000000116 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: 418.31 deg C (estimated)) (Using MP: 173.09 deg C (estimated)) VP: 1.28E-008 mm Hg (Antoine Method) VP: 8.7E-008 mm Hg (Modified Grain Method) VP: 2.11E-007 mm Hg (Mackay Method) Selected VP: 8.7E-008 mm Hg (Modified Grain Method)
Reliability:	(2) valid with restrictions Accepted calculation method
Flag:	Critical study for SIDS endpoint

28-SEP-2001 (1)

2.5 Partition Coefficient

log Pow: 1.59
Method: other (calculated): KOWWIN Program (v1.65)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
28-SEP-2001 (1)

2.6.1 Water Solubility

Value: 657.6 mg/l at 25 degree C
Method: other: (WSKOW v1.36)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Remark: Log Kow used by Water solubility estimates: 1.59

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
28-SEP-2001 (1)

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: .0000000003449482 cm3/(molecule * sec)
Degradation: 50 % after .4 hour(s)
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
28-SEP-2001 (1)

3.1.2 Stability in Water

Type: abiotic
Method:
Year: GLP:
Test substance:
Remark: See IUCLID documents on CAS #149-30-4 and #120-78-5
09-OCT-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:

	Distribution (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	0.000176	0.744	1000	2.94e-015
Water	36.6	900	1000	1.43e-016
Soil	63.3	900	1000	4.01e-015
Sediment	0.0926	3.6e+003	0	1.3e-016

Persistence Time: 879 hr
Reaction Time: 1.3e+003 hr

Advection Time: 2.73e+003 hr
Percent Reacted: 67.8
Percent Advected: 32.2
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
09-OCT-2001 (1)

3.3.2 Distribution
-

3.4 Mode of Degradation in Actual Use
-

3.5 Biodegradation

Type: aerobic
Inoculum:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID documents on CAS #149-30-4 and #120-78-5
09-OCT-2001

3.6 BOD5, COD or BOD5/COD Ratio
-

3.7 Bioaccumulation

Species: other: calculation
Exposure period:
Concentration:
BCF: 3.37
Elimination:
Method: other: BCF Program (v2.13)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Result: Log Kow (estimated) : 1.59
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 1.59

Equation Used to Make BCF estimate:
Log BCF = 0.77 log Kow - 0.70

Estimated Log BCF = 0.528 (BCF = 3.369)
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
28-SEP-2001 (1)

3.8 Additional Remarks
-

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: other: calculated
Species: other: fish
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: 512.09
Method: other: (calculated) ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
28-SEP-2001 (1)

Type: other: calculated
Species: other: fish
Exposure period: 14 day
Unit: mg/l Analytical monitoring: no
LC50: 869.073
Method: other: (calculated) ECOSAR v0.99e
Year: GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
28-SEP-2001 (1)

Type: other
Species:
Exposure period:
Unit: Analytical monitoring:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID documents on CAS #149-30-4 and #120-78-5
09-OCT-2001

4.2 Acute Toxicity to Aquatic Invertebrates

Type: other: calculated
Species: Daphnia sp. (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 533.392
Method: other: (calculated) ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
09-OCT-2001 (1)

Type: other: calculated
Species: Mysidopsis bahia (Crustacea)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50 : 197.9
Method: other: (calculated) ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
28-SEP-2001 (1)

Type:
Species:
Exposure period:
Unit: Analytical monitoring:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID documents on CAS #149-30-4 and #120-78-5
09-OCT-2001

Type: other: calculated
Species: Daphnia magna (Crustacea)
Exposure period: 16 day
Unit: mg/l Analytical monitoring: no
EC50: 22.864
Method: other: (calculated) ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
28-SEP-2001 (1)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: other algae: green algae
Endpoint: growth rate
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 325.584
Method: other: (calculated) ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Remark: Chronic value = 25.697 mg/l (96 hr)
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
28-SEP-2001 (1)

Species:
Endpoint:
Exposure period:
Unit: Analytical monitoring:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID documents on CAS #149-30-4 and #120-78-5
09-OCT-2001

4.4 Toxicity to Microorganisms e.g. Bacteria
-

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

Species: other: fish
Endpoint:
Exposure period: 30 day
Unit: mg/l Analytical monitoring: no
ChV : 61.751
Method: other: (calculated) ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
28-SEP-2001 (1)

4.5.2 Chronic Toxicity to Aquatic Invertebrates
-

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms

Type:	other: calculated
Species:	Eisenia fetida (Worm (Annelida), soil dwelling)
Endpoint:	
Exposure period:	14 day
Unit:	other: mg/l
LC50:	2340.056
Method:	other: (calculated) ECOSAR v0.99e
Year:	1999 GLP: no
Test substance:	other TS: molecular structure
Reliability:	(2) valid with restrictions Accepted calculation method

28-SEP-2001 (1)

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: other
Species:
Strain:
Sex:
Number of Animals:
Vehicle:
Value:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID documents on CAS #149-30-4 and #120-78-5
09-OCT-2001

5.1.2 Acute Inhalation Toxicity

-

5.1.3 Acute Dermal Toxicity

Type: other
Species:
Strain:
Sex:
Number of Animals:
Vehicle:
Value:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID documents on CAS #149-30-4 and #120-78-5
09-OCT-2001

5.1.4 Acute Toxicity, other Routes

-

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation
-

5.2.2 Eye Irritation
-

5.3 Sensitization
-

5.4 Repeated Dose Toxicity

Species: Sex:
Strain:
Route of admin.:
Exposure period:
Frequency of treatment:
Post. obs. period:
Doses:
Control Group:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID documents on CAS #149-30-4 and #120-78-5
09-OCT-2001

5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: Salmonella typhimurium, strains TA-1535, TA-1537, TA-98, TA-100
Concentration: 0.1,1.0,10,100,1000 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year: GLP: no data
Test substance: other TS: CAS# 95-32-9, purity = 96.1%
Result: Cytotoxicity concentrations:
With metabolic activation = 100 ug/ plate
Without metabolic activation = 100-100 ug/ plate
(based on zero to low number revertants per plate)
Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint

28-SEP-2001 (2)

Type: Mammalian cell gene mutation assay
System of testing: Clone I-13 of BALB 3T3 mouse cells
Concentration: 0.01, 0.1, 0.5, 1.0, 2.0 ug/ml
Cytotoxic Conc.: 26.7% survival at 3.91 ug/l; no survivors at 7.81 ug/l
Metabolic activation: without
Result: negative
Method: other: Litton Bionetics Assay Design No. 441
Year: GLP: yes
Test substance: other TS: Morfax
Remark: Cytotoxicity concentration:
80-20% survival over test range.
Precipitation concentration:
slight turbidity noted at 1.0 mg/ml stock solution, but not in lower concentrations obtained by serial dilution; none noted in test concentrations.
Reliability: (2) valid with restrictions
GLP guideline study
Flag: Critical study for SIDS endpoint
28-SEP-2001 (3)

5.6 Genetic Toxicity 'in Vivo'

Type:
Species: Sex:
Strain:
Route of admin.:
Exposure period:
Doses:
Result:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID documents on CAS #149-30-4 and #120-78-5
09-OCT-2001

5.7 Carcinogenicity

Species: other Sex:
Strain:
Route of admin.:
Exposure period:
Frequency of
treatment:
Post. obs.
period:
Doses:
Result:
Control Group:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID documents on CAS #149-30-4 and #120-78-5
09-OCT-2001

5.8 Toxicity to Reproduction

Type: other
Species: Sex:
Strain:
Route of admin.:
Exposure Period:
Frequency of
treatment:
Duration of test:
Doses:
Control Group:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID documents on CAS #149-30-4 and #120-78-5
09-OCT-2001

5.9 Developmental Toxicity/Teratogenicity

Species: Sex:
Strain:
Route of admin.:
Exposure period:
Frequency of
treatment:
Duration of test:
Doses:
Control Group:
Method:
Year: GLP:
Test substance:
Remark: See IUCLID documents on CAS #149-30-4 and #120-78-5
09-OCT-2001

5.10 Other Relevant Information
-

5.11 Experience with Human Exposure
-

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

(2) The Goodyear Tire & Rubber Company, Laboratory report No. 79-76, Mutagenicity Evaluation of WTR No. 23e, January 25, 1980.

(3) Litton Bionetics, Inc. Project No 20992. January, 1981. submitted to The Goodyear Tire & Rubber Company.

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: 120-78-5
CAS No.	120-78-5
EINECS Name	di(benzothiazol-2-yl) disulphide
EINECS No.	204-424-9
TSCA Name	Benzothiazole, 2,2'-dithiobis-
Molecular Formula	C14H8N2S4

Producer Related Part	
Company:	
Creation date:	06-NOV-2000

Substance Related Part	
Company:	
Creation date:	06-NOV-2000

Memo:	Data for RAPA Benzothiazole-based Thiazoles category

Printing date:	09-OCT-2001
Revision date:	
Date of last Update:	26-APR-2001

Number of Pages:	67

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
-

1.0.2 Location of Production Site
-

1.0.3 Identity of Recipients
-

1.1 General Substance Information
-

1.1.0 Details on Template
-

1.1.1 Spectra
-

1.2 Synonyms
-

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: 180 degree C
Method: other: Handbook value
Testsubstance: other TS: purity not noted
Source: Bayer AG Leverkusen
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
26-APR-2001 (1)

Value: 168 degree C
Source: Bayer AG Leverkusen
19-APR-1993 (2)

Value: > 169 degree C
Source: Bayer AG Leverkusen
02-APR-1993 (3)

Value: 170 degree C
Source: Monsanto
Bayer AG Leverkusen
10-MAY-1994 (4)

Value: 180 - 182 degree C
Source: Bayer AG Leverkusen
19-APR-1993 (5)

2.2 Boiling Point

Value:
Decomposition: yes
Source: Bayer AG Leverkusen
Reliability: (2) valid with restrictions
06-NOV-2000 (2)

2.3 Density

Type: density
Value: 1.54 at 25 degree C
Method: other: Handbook value
Testsubstance: other TS: purity not noted
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
26-APR-2001 (6)

Type: density
Value: 1.34 g/cm3 at 20 degree C
Source: Bayer AG Leverkusen
02-APR-1993 (3)

Type: density
Value: 1.5 g/cm3 at 20 degree C
Source: Bayer AG Leverkusen
19-APR-1993 (2) (1)

Type: density
Value: ca. 1.51 g/cm3 at 20 degree C
Source: Bayer AG Leverkusen
02-APR-1993 (7)

2.3.1 Granulometry
-

2.4 Vapour Pressure

Value: .000000000597 hPa at 20 degree C
Method: OECD Guide-line 104 "Vapour Pressure Curve"
GLP: yes
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
06-NOV-2000 (8)

Value: .0000000543 hPa at 50 degree C
Method: OECD Guide-line 104 "Vapour Pressure Curve"
GLP: yes
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
06-NOV-2000 (8)

Value:
Remark: value:
< 2 x 10 exp -6 torr
Source: Monsanto
Bayer AG Leverkusen
26-APR-2001 (9)

2.5 Partition Coefficient

log Pow: 4.5
Method: other (measured): flask shaking method
Year: 1980
GLP: no
Source: Bayer AG Leverkusen
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
06-NOV-2000 (10)

log Pow: 4.5
Method: other (calculated)
Year:
Source: Bayer AG Leverkusen
06-NOV-2000 (9)

log Pow: 4.659 at 25 degree C
Method: other (calculated)
Year:
Flag: Critical study for SIDS endpoint
26-APR-2001 (11)

2.6.1 Water Solubility

Value: 80 - 96 mg/l at 22 degree C
pH: 5
Method: other
Remark: Value: 88 +/- 8 mg/l
Temperature: 22 °C
pH: 5
Elution through a glass bed column proviously coated with MBTS; HPLC measurement
Value: 49 +/- 2 mg/l at pH 9
Source: Bayer AG Leverkusen
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
06-NOV-2000 (12)

Value: 68 other: ppm at 22 degree C
Method: other: calculated
06-NOV-2000 (13)

Value: < .0002 g/l at 20 degree C
Source: Bayer AG Leverkusen
09-AUG-1993 (8)

Value: < 1 g/l at 21 degree C
Source: Bayer AG Leverkusen
29-APR-1993 (2)

Value: < 10 mg/l
Source: Bayer AG Leverkusen
11-AUG-1993 (14)

2.6.2 Surface Tension
-

2.7 Flash Point

Value: 257 degree C
Type: closed cup
Method: other: DIN 51758
Year:
Source: Bayer AG Leverkusen
02-APR-1993 (3)

Value: 271 degree C
Type:
Method:
Year:
Source: Bayer AG Leverkusen
19-APR-1993 (2)

2.8 Auto Flammability
-

2.9 Flammability
-

2.10 Explosive Properties
-

2.11 Oxidizing Properties
-

2.12 Additional Remarks

Remark: Ignition temperature: > 365 degree C
Source: Bayer AG Leverkusen
30-APR-1993 (3)

3.1.1 Photodegradation

Type: water
Light source: Sun light
DIRECT PHOTOLYSIS
Halflife t1/2: 3 hour(s)
Method:
Year: GLP:
Test substance: other TS: MBTS purity = 98%
Remark: dark control 19 hours
Source: Bayer AG Leverkusen
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
26-APR-2001 (15)

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1560000 molecule/cm3
Rate constant: .0000000003152585 cm3/(molecule * sec)
Degradation: 50 % after 24.4 minute(s)
Method: other (calculated): AOP Program (v1.89)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Flag: Critical study for SIDS endpoint
26-APR-2001 (11)

Type: air
INDIRECT PHOTOLYSIS
Rate constant: .0000000002 cm3/(molecule * sec)
Degradation: 50 % after 1.9 hour(s)
Method: other (calculated): according to Atkinson
Year: 1990 GLP:
Test substance:
Remark: no direct photolysis; sensitizer: OH-radicals
Source: Bayer AG Leverkusen
25-MAY-1993 (16)

Type:
Method:
Year: GLP:
Test substance:
Remark: UV-irradiation of bis-(2-benzothiazolyl)-disulfide (2.5 g, 7.5 mmol) in acetonitrile or ethanol (120 h) gave following products: Benzothiazole (6.8%), elemental sulphur (14.2%), 2(3H)-benzothiazolethione (29.2%), bis-(2-benzo-thiazolyl)-disulfide (17.0%), 2(3H)-benzothiazolone (30.0%).
Source: Bayer AG Leverkusen
09-JUN-1993 (17)

3.1.2 Stability in Water

Type: abiotic
Degradation: 37 % after 7 day
at pH 7
Method:
Year: GLP:
Test substance: other TS: MBTS purity = 98%
Remark: Thiofide hydrolized approximately 37% after a 7-day period in pH 7 buffered deionized water with light excluded. The sole hydrolysis product indentified was mercaptobenzthiazole.
Source: Bayer AG Leverkusen
Reliability: (2) valid with restrictions
06-NOV-2000 (18)

Type: abiotic
Method:
Year: GLP:
Test substance:
Remark: Hydrolysis to 2-Mercaptobenzothiazole and Benzothiazyl-2-sulfenic acid; further reaction of the sulfenic acid to 2,2'-Dithiobisbenzothiazole, Benzothiazyl-2-sulfinic acid and Benzothiazyl-2-sulfonic acid (no other information).
Source: Bayer AG Leverkusen
06-JAN-1994 (5)

Type: abiotic
Method:
Year: GLP:
Test substance:
Remark: Alkalic hydrolysis (pH 9.8-12.1) to 2-Mercaptobenzothiazole and Benzothiazyl-2-sulfenic acid; further reaction of the sulfenic acid to 2-Mercaptobenzothiazole, Benzothiazyl-2-sulfinic acid and Benzothiazyl-2-sulfonic acid. In the presence of oxidizing agents 2-Mercaptobenzothiazole reacts to MBTS, Benzothiazyl-2-sulfinic acid will be oxidized to the sulfonic acid. Based on a cyclic process Benzothiazyl-2-sulfonic acid is the major hydrolysis product of MBTS.
Source: Bayer AG Leverkusen
13-MAY-1993 (19)

3.1.3 Stability in Soil

Type: Radiolabel:
Concentration:
Cation exch.
capac.
Microbial
biomass:
Method:
Year: GLP:
Test substance:
Remark: no information
Source: Bayer AG Leverkusen
05-AUG-1992

3.2 Monitoring Data (Environment)

Type of
measurement: background concentration
Medium: other: surface water and sediment
Method:
Concentration
Remark: MBTS was not detected in 42 samples in Japan in 1978;
detection limit: - water: 0.5 ug/l
- sediment: 0.05 - 0.17 mg/kg
Source: Bayer AG Leverkusen
11-AUG-1993 (20)

Type of
measurement: concentration at contaminated site
Medium: other: waste water from MBTS production sites, USA
Method:
Concentration
Remark: untreated effluent: 0.5 - 10 ppm (no further information)
Source: Bayer AG Leverkusen
09-JUN-1993 (21)

Type of
measurement: concentration at contaminated site
Medium: other: effluent from a publicly owned treatment plant,
handling effluents from a plant manufacturing MBTS, USA
Method:
Concentration
Remark: average concentration: 11 ug/l (4 samples)
Source: Bayer AG Leverkusen
09-JUN-1993 (21)

Type of measurement:
Medium:
Method:
Concentration
Remark: no information (Germany)
Source: Bayer AG Leverkusen
05-AUG-1992

3.3.1 Transport between Environmental Compartments

Type:
Media: other: soil-air, water-air, water-soil
Air (Level I):
Water (Level I):
Soil (Level I):
Biota (L.II/III):
Soil (L.II/III):
Method:
Year:
Remark: Based on the physico-chemical properties transport between air and water/soil has to be expected to a small extent
Source: Bayer AG Leverkusen
25-MAY-1993

3.3.2 Distribution

Media: air - biota - sediment(s) - soil - water
Method: Calculation according Mackay, Level III
Year: 1999
Result:

	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	0.00014	0.814	1000	7.01e-017
Water	17.2	900	1000	1.98e-018
Soil	72.7	900	1000	2.14e-019
Sediment	10.2	3.6e+003	0	1.35e-018

Persistence Time: 1.13e+003 hr
Reaction Time: 1.4e+003 hr
Advection Time: 5.76e+003 hr
Percent Reacted: 80.4
Percent Advecte
Reliability: (2) valid with restrictions
06-NOV-2000 (11)

Media:
Method:
Year:
Remark: no information
Source: Bayer AG Leverkusen
05-AUG-1992

3.4 Mode of Degradation in Actual Use

Remark: no information
Source: Bayer AG Leverkusen
05-AUG-1992

3.5 Biodegradation

Type: aerobic
Inoculum: other: activated sludge, predominantly industrial waste water, adapted
Concentration: 100 mg/l related to Test substance
Degradation: 2 % after 28 day
Result: other: not readily biodegradable
Method: other: Manometrischer Respirationstest, Verfahren nach Richtlinie 79/831/EWG, Anhang V, Teil C (aktualisierte Fassung vom Juli 1990), Methode C.4-D
Year: 1992 GLP: yes
Test substance: other TS: purity 97.8 %
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
06-NOV-2000 (8)

Type: aerobic
Inoculum: activated sludge, domestic
Concentration: 100 mg/l related to Test substance
Degradation: 0 % after 28 day
Result: under test conditions no biodegradation observed
Method: other: MITI-Test OECD-Test Guideline 301 C; according to the EC-method: Assessment of Biodegradability of Chemicals in Water by Manometric Respirometry (DG X 1 283/82 Rev. 5)
Year: 1988 GLP: yes
Test substance: other TS: technical grade
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
06-NOV-2000 (8)

Type: aerobic
Inoculum: activated sludge, non-adapted
Concentration: 100 mg/l related to Test substance
Degradation: .8 % after 14 day
Method: other: see remarks
Year: GLP: no data
Test substance: other TS: MBTS (no information about purity)
Remark: sludge concentration: 30 mg/l
method:
"Biodegradation test of chemical substance by microorganisms etc." stipulated in the Order Prescribing the Items of the Test Relating to the New Chemical Substance (1974, Order of the Prime Minister, Minister of Health and Welfare, the MITI No. 1). This guideline corresponds to "301C, Ready Biodegradability: Modified MITI Test I" stipulated in the OECD Guideline for Testing of Chemicals (May 12, 1981).
Source: Bayer AG Leverkusen
06-NOV-2000 (14)

3.6 BOD5, COD or BOD5/COD Ratio

Remark: COD: 1973 mg/g
Source: Bayer AG Leverkusen
28-MAY-1993 (8)

3.7 Bioaccumulation

Species: Cyprinus carpio (Fish, fresh water)
Exposure period: 42 day at 25 degree C
Concentration: .2 mg/l
BCF: 1 - 7.2
Elimination: no data
Method: other: see remarks
Year: GLP: no data
Test substance: other TS: MBTS (no information about purity
Remark: method:
"Bioaccumulation test of chemical substance in fish and shellfish" stipulated in the Order Prescribing the Items of the Test Relating to the New Chemical Substance (1974, Order of the Prime Minister, Minister of Health and Welfare, the MITI No. 1). This guideline corresponds to "305C, Bio-accumulation: Degree of Bioconcentration in Fish" stipulated in the OECD Guidelines for Testing of Chemicals (May 12, 1981).
Source: Bayer AG Leverkusen
11-AUG-1993 (14)

Species: Cyprinus carpio (Fish, fresh water)
Exposure period: 42 day at 25 degree C
Concentration: .02 mg/l
BCF: < 1.4 - 51
Elimination: no data
Method: other: see remarks
Year: GLP: no data
Test substance: other TS: MBTS (no information about purity)
Remark: method:
"Bioaccumulation test of chemical substance in fish and shellfish" stipulated in the Order Prescribing the Items of the Test Relating to the New Chemical Substance (1974, Order of the Prime Minister, Minister of Health and Welfare, the MITI No. 1). This guideline corresponds to "305C, Bio-accumulation: Degree of Bioconcentration in Fish" stipulated in the OECD Guidelines for Testing of Chemicals (May 12, 1981).
Source: Bayer AG Leverkusen
11-AUG-1993 (14)

3.8 Additional Remarks
-

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: static
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: 66
Method:
Year: GLP: no data
Test substance: other TS: MBTS purity =98%
Source: Monsanto
Bayer AG Leverkusen
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
06-NOV-2000 (22)

Type: static
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: > 1000
Method:
Year: GLP: no data
Test substance: other TS: MBTS purity =98%
Source: Monsanto
Bayer AG Leverkusen
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
06-NOV-2000 (23)

Type: other: calculated
Species: other
Exposure period: 14
Unit: mg/l Analytical monitoring: no
LC50: 2.152
Method: other: ECOSAR Program (v0.99e)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
26-APR-2001 (11)

Type: other: calculated
Species: other
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: .779
Method: other: ECOSAR Program (v0.99e)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
26-APR-2001 (11)

Type:
Species: Lepomis macrochirus (Fish, fresh water)
Exposure period:
Unit: mg/l Analytical monitoring:
LC50: 82
Method:
Year: GLP:
Test substance:
Source: Monsanto
Bayer AG Leverkusen
10-MAY-1994 (24)

Type:
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period: 13 day
Unit: Analytical monitoring:
Method:
Year: GLP:
Test substance:
Remark: In a time-independent test rainbow trout was exposed to MBTS acutely. No mortality was noted in the fish over the 13 day study period at exposure values up to 15 mg/l, the highest level tested in the study. Based on the data, MBTS was judged to not be highly toxic to the fish following acute exposure.
Source: Monsanto
Bayer AG Leverkusen
10-MAY-1994 (25)

Type:
Species: Oryzias latipes (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no data
LC50: 19
Method: other: Japanese Industrial Standard (JIS K 0102-1986-71) "Testing methods for industrial waste water"
Year: GLP: no data
Test substance: other TS: MBTS (no information about purity)
Source: Bayer AG Leverkusen
11-AUG-1993 (14)

4.2 Acute Toxicity to Aquatic Invertebrates

Type:
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: Analytical monitoring: yes
Method: other: Pruefrichtlinie "Akute Toxizitaet fuer Daphnien (C.2) Richtlinie 67/548/EWG (Entwurf 1992)
Year: 1992 GLP: yes
Test substance: other TS: purity 97.8 %
Remark: No immobilization within the range of water solubility, effects could be observed only for test concentration above water solubility.
Used analytical method could not verify testing concentration.
Analytical monitoring: HPLC
Source: Bayer AG Leverkusen
Test condition: Ultra-Turrax stirred for 60 sec
pH 8.0 - 8.2
Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
06-NOV-2000 (8)

Type:
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring:
EC50: 82
Method:
Year: GLP: no data
Test substance: other TS: MBTS purity =98%
Source: Monsanto
Bayer AG Leverkusen
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
06-NOV-2000 (26)

Type: other: calculated
Species: Daphnia sp. (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 1.003
Method: other: ECOSAR Program (v0.99e)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
26-APR-2001 (11)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Scenedesmus subspicatus (Algae)
Endpoint: other: growth rate, biomass
Exposure period: 72 hour(s)
Unit: Analytical monitoring: no
Method: other: Pruefrichtlinie "Algeninhibitionstest" (C.3) Richtlinie 67/548/EWG (Entwurf 1992)
Year: 1992 GLP: yes
Test substance: other TS: purity 97.8 %
Remark: No growth inhibition of the population tested within the range of water solubility of the substance. The only tested concentration was 40 mg/l, pH 8.1 - 10.3
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
06-NOV-2000 (8)

Species: other algae
Endpoint: other: cell count
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
EC50: .6
Method:
Year: GLP:
Test substance: other TS: MBTS purity = 98%
Remark: Sharen - check if 0.06 or 0.6 mg/l
Source: Monsanto
Bayer AG Leverkusen
06-NOV-2000 (27)

Species: other algae
Endpoint: other: chlorophyll a
Exposure period:
Unit: mg/l Analytical monitoring:
EC50: .7
Method:
Year: GLP:
Test substance: other TS: MBTS purity = 98%
Source: Monsanto
Bayer AG Leverkusen
06-NOV-2000 (27)

Species: other algae: green algae
Endpoint: growth rate
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: c .731
ChV : c .34
Method: other: ECOSAR Program (v0.99e)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
26-APR-2001 (11)

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: > 10000
Method: other: Test for Inhibition of Oxygen Consumption by Activated Sludge, ISO 8192
Year: 1988 GLP: yes
Test substance: other TS: technical grade
Remark: Direct weight, 6 mg/l inoculum (dry weight) from a laboratory bench-scale system
Source: Bayer AG Leverkusen
11-AUG-1993 (8)

Type: aquatic
Species: activated sludge
Exposure period:
Unit: mg/l Analytical monitoring: no data
EC75 : 38
Method: other: quantitative determination of the nitrification rate, colorimetric measurement of the NO2/NO3-concentration; static test system
Year: GLP: no
Test substance:
Remark: Pre-cleaned activated sludge in particle-free communal waste water (BSB5: 250 mg/l; NH4-N/l: 50-80 mg/l); determination of the effective concentration which caused a decrease of the 1st step of the nitrification rate (NH4 to NO2) of 75 %. Exposure period: 2-4 h.
Source: Bayer AG Leverkusen
Test condition: 25 degree C; pH 7.6-7.8
02-JUN-1993 (28)

Type: aquatic
Species: activated sludge, industrial
Exposure period: 4 hour(s)
Unit: mg/l Analytical monitoring: no data
EC50: 60
Method: other: Inhibition of cell reproduction; static test system; colorimetric measurement
Year: GLP: no data
Test substance:
Source: Bayer AG Leverkusen
Test condition: 37 degree C; pH 7
02-JUN-1993 (29)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

Species: other
Endpoint: other
Exposure period: 30 day
Unit: mg/l Analytical monitoring: no
ChV : c .154
Method: other: ECOSAR Program (v0.99e)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
26-APR-2001 (11)

4.5.2 Chronic Toxicity to Aquatic Invertebrates

Species: Daphnia sp. (Crustacea)
Endpoint: other
Exposure period: 16 day
Unit: mg/l Analytical monitoring: no
EC50: .165
Method: other: ECOSAR Program (v0.99e)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
26-APR-2001 (11)

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms

Type:
Species: Eisenia fetida (Worm (Annelida), soil dwelling)
Endpoint:
Exposure period: 14 day
Unit: other: ppm
LC50: 310.082
Method: other: ECOSAR Program (v0.99e)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Remark: Chemical may not be soluble enough to measure this predicted effect.
Reliability: (2) valid with restrictions
26-APR-2001 (11)

4.6.2 Toxicity to Terrestrial Plants

Species:
Endpoint:
Expos. period:
Unit:
Method:
Year: GLP:
Test substance:
Remark: no information
Source: Bayer AG Leverkusen
05-AUG-1992

4.6.3 Toxicity to other Non-Mamm. Terrestrial Species
-

4.7 Biological Effects Monitoring

Remark: no information
Source: Bayer AG Leverkusen
05-AUG-1992

4.8 Biotransformation and Kinetics

Type:
Remark: no information
Source: Bayer AG Leverkusen
05-AUG-1992

4.9 Additional Remarks

Remark: Soil fungi, growth inhibition test:
4 d LD50 = 0.5 % related to the growth of the control
14 d LD50 = 0.75 % related to the growth of the control
Test Condition: 25 degree C, aqueous soil extract, no data on concentrations used in the test, test substance incorporated in nutrient agar
Source: Bayer AG Leverkusen
25-MAY-1993 (30)

Remark: Soil fungi:
Species: Fusarium oxysporum sp. albedinis
Growth inhibition after 5 days, test substance concentration:
41.5 mg/l = 6 %
133 mg/l = 100 %
Source: Bayer AG Leverkusen
30-APR-1993 (31)

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type:	LD50
Species:	rat
Strain:	
Sex:	
Number of Animals:	
Vehicle:	other: corn oil
Value:	> 7940 mg/kg bw
Method:	other
Year:	GLP: no data
Test substance:	other TS: MBTS purity 98%; 25 % solution in corn oil
Remark:	method: 7 animals tested remark: signs of intoxication: reduced appetite and activity one to three days; no mortality; viscera appeared normal
Source:	Bayer AG Leverkusen
Reliability:	(2) valid with restrictions

06-NOV-2000 (32)

Type:	LD50
Species:	rat
Strain:	
Sex:	
Number of Animals:	
Vehicle:	
Value:	= 7000 mg/kg bw
Method:	
Year:	GLP: no data
Test substance:	no data
Remark:	method: no data
Source:	Bayer AG Leverkusen

22-APR-1993 (33)

Type:	LD50
Species:	rat
Strain:	
Sex:	
Number of Animals:	
Vehicle:	
Value:	> 7000 mg/kg bw
Method:	
Year:	GLP: no data
Test substance:	no data
Remark:	method: no data
Source:	Bayer AG Leverkusen

22-APR-1993 (34)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 433 mg/kg bw
Method:
Year: GLP: no data
Test substance: no data
Remark: method: no data
Source: Bayer AG Leverkusen
11-APR-1995 (35)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 12000 mg/kg bw
Method:
Year: GLP: no data
Test substance: no data
Remark: method: no data
Source: Bayer AG Leverkusen
22-APR-1993 (36)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: > 5000 mg/kg bw
Method:
Year: GLP: no data
Test substance: no data
Remark: method: no data
remarks: mortality: 0/10
Source: Bayer AG Leverkusen
22-APR-1993 (37)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: ca. 7000 mg/kg bw
Method:
Year: GLP: no data
Test substance: no data
Remark: method: no data
Source: Bayer AG Leverkusen
22-APR-1993 (38)

Type:
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: 5000 - 8000 mg/kg bw
Method: other
Year: GLP: no data
Test substance: other TS: 40 % suspension in corn oil
Remark: method: 48 animals tested
remarks: no signs of intoxication
Source: Bayer AG Leverkusen
13-MAY-1993 (39)

Type: LD50
Species: mouse
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 7000 mg/kg bw
Method:
Year: GLP: no data
Test substance: no data
Remark: method: no data
Source: Bayer AG Leverkusen
22-APR-1993 (34)

Type: LD50
Species: mouse
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: = 4631 mg/kg bw
Method:
Year: GLP: no data
Test substance: no data
Remark: method: no data
Source: Bayer AG Leverkusen
11-APR-1995 (35)

Type: LD50
Species: mouse
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: = 12000 mg/kg bw
Method:
Year: GLP: no data
Test substance: no data
Remark: method: no data
Source: Bayer AG Leverkusen
22-APR-1993 (36)

Type: LD50
Species: mouse
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: > 3370 mg/kg bw
Method:
Year: GLP: no data
Test substance: no data
Remark: method: no data
Source: Bayer AG Leverkusen
22-APR-1993 (40)

Type: LD0
Species: mouse
Strain:
Sex:
Number of Animals:
Vehicle:
Value: < 2000 mg/kg bw
Method: other
Year: GLP: no data
Test substance: other TS: 40 % suspension in corn oil
Remark: mortality: 3/24 animals
Source: Bayer AG Leverkusen
13-MAY-1993 (39)

Type: LD50
Species: rabbit
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 6200 mg/kg bw
Method:
Year: GLP: no data
Test substance: no data
Remark: method: no data
Source: Bayer AG Leverkusen
11-APR-1995 (35)

Type: LD0
Species: guinea pig
Strain:
Sex:
Number of Animals:
Vehicle:
Value: < 4000 mg/kg bw
Method: other
Year: GLP: no data
Test substance: other TS: 40 % suspension in corn oil
Remark: mortality: 2/8 animals
Source: Bayer AG Leverkusen
13-MAY-1993 (39)

5.1.2 Acute Inhalation Toxicity
-

5.1.3 Acute Dermal Toxicity

Type:	LD50
Species:	rabbit
Strain:	
Sex:	
Number of Animals:	
Vehicle:	
Value:	> 7940 mg/kg bw
Method:	other
Year:	GLP: no data
Test substance:	other TS: MBTS purity 98%
Remark:	method: 3 animals tested remarks: reduced appetite and activity in 1 to 2 d; no mortality; viscera appeared normal
Source:	Bayer AG Leverkusen
Reliability:	(2) valid with restrictions

06-NOV-2000 (41)

5.1.4 Acute Toxicity, other Routes

Type:	LD50
Species:	rat
Strain:	
Sex:	
Number of Animals:	
Vehicle:	
Route of admin.:	i.p.
Value:	= 2600 mg/kg bw
Method:	
Year:	GLP: no data
Test substance:	no data
Remark:	method: no data
Source:	Bayer AG Leverkusen

22-APR-1993 (34)

Type:	LD50
Species:	rat
Strain:	
Sex:	
Number of Animals:	
Vehicle:	
Route of admin.:	i.p.
Value:	= 3000 mg/kg bw
Method:	
Year:	GLP: no data
Test substance:	no data
Remark:	method: no data
Source:	Bayer AG Leverkusen

22-APR-1993 (34)

Type: LD50
Species: mouse
Strain:
Sex:
Number of
Animals:
Vehicle:
Route of admin.: i.p.
Value:
Method:

Year: GLP: no data
Test substance: other TS: only code designations are given (B-23, EK-5432, Y-5)
Remark: method: no data
remarks: mortality not reported
value: > 2000 mg/kg; 100-200 mg/kg
Source: Bayer AG Leverkusen
11-APR-1995 (42)

Type: LD50
Species: mouse
Strain:
Sex:
Number of
Animals:
Vehicle:
Route of admin.: i.p.
Value: = 2250 mg/kg bw
Method:
Year: GLP: no data
Test substance: no data
Remark: method: no data
Source: Bayer AG Leverkusen
22-APR-1993 (40)

Type: LD50
Species: mouse
Strain:
Sex:
Number of
Animals:
Vehicle:
Route of admin.: i.v.
Value: = 180 mg/kg bw
Method:
Year: GLP: no data
Test substance: no data
Remark: method: no data
Source: Bayer AG Leverkusen
22-APR-1993 (43)

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: other: see remarks
Year: GLP: no data
Test substance: no data
Remark: method: 10 g/kg was applied to the skin for 24 h
Source: Bayer AG Leverkusen
22-APR-1993 (38)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result: not irritating
EC classificat.:
Method: other: Federal Hazardous Substances Act
Year: GLP: no data
Test substance: other TS: Purity = 98%
Remark: method: 0.5 g/animal (moistened with water) was applied to the skin for 24 h
Source: Bayer AG Leverkusen
26-APR-2001 (44)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result:
EC classificat.:
Method: Draize Test
Year: GLP: no data
Test substance: no data
Remark: 4 animals tested
result: according to authors: mild irritant
Source: Bayer AG Leverkusen

13-MAY-1993 (40)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result: not irritating
EC classificat.:
Method:
Year: GLP:
Test substance:
Remark: 0.0/8.0
Source: Monsanto
Bayer AG Leverkusen

10-MAY-1994 (45)

Species: human
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result:
EC classificat.:
Method: other: application of dry form or oil solution to the skin of 6 persons for 24 h
Year: GLP: no data
Test substance: no data
Remark: no symptoms were observed
Source: Bayer AG Leverkusen

22-APR-1993 (46)

Species: human
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result:
EC classificat.:
Method: other: repeated insult patch test (see also chapter 5.3)
Year: GLP: no data
Test substance: no data
Remark: The result of the first application indicated that MBTS was incapable of acting as primary irritant of the immediate type in any of the 53 individuals under test.
Source: Bayer AG Leverkusen

22-APR-1993 (47)

5.2.2 Eye Irritation

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result:
EC classificat.:
Method: Draize Test
Year: GLP: no data
Test substance: no data
Remark: 4 animals tested
result: according to authors: strongly irritating
Source: Bayer AG Leverkusen
13-MAY-1993 (40)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: slightly irritating
EC classificat.:
Method: other: Federal Hazardous Substances Act
Year: GLP: no data
Test substance: no data
Remark: method: 100 mg/animal were applied as finely ground powder to the eyes
Source: Bayer AG Leverkusen
22-APR-1993 (48)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: not irritating
EC classificat.:
Method:
Year: GLP:
Test substance:
Remark: 0.6/110.0
Source: Monsanto
Bayer AG Leverkusen
10-MAY-1994 (45)

5.3 Sensitization

Type:	Guinea pig maximization test
Species:	guinea pig
Number of Animals:	
Vehicle:	
Result:	
Classification:	
Method:	other: original procedure of Magnusson & Klingman with some modifications
Year:	GLP: no data
Test substance:	other TS: serial dilutions in petrolatum
Remark:	A new protocol and criteria for quantitative evaluation of sensitization potencies is presented. Known sensitizers (e.g. MBTS) are tested by changing the application concentrations for induction as well as for challenge
Source:	Bayer AG Leverkusen

22-JAN-1996 (49)

Type:	Guinea pig maximization test
Species:	guinea pig
Number of Animals:	
Vehicle:	
Result:	sensitizing
Classification:	
Method:	
Year:	GLP:
Test substance:	
Source:	Bayer AG Leverkusen

02-APR-1993 (50)

Type:	Patch-Test
Species:	human
Number of Animals:	
Vehicle:	
Result:	
Classification:	
Method:	other
Year:	GLP: no data
Test substance:	other TS: 1% in petrolatum
Remark:	11/46 patients with occupational rubber dermatitis had a positive patch test result with MBTS
Source:	Bayer AG Leverkusen

19-JAN-1996 (51)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method: other
Year: GLP: no data
Test substance: other TS: 2% in Eucerin
Remark: 1/2 patients with rubber dermatitis had a positive patch test result with MBTS
Source: Bayer AG Leverkusen
19-JAN-1996 (52)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method: other
Year: GLP: no data
Test substance: other TS: 1% in petrolatum
Remark: 29/686 rubber sensitized patients had a positive patch test result with MBTS
Source: Bayer AG Leverkusen
19-JAN-1996 (53)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method: other
Year: GLP: no data
Test substance: other TS: serial dilutions (1-0.0032%) in petrolatum
Remark: 12 rubber-sensitive subjects were tested, significant differences from none in response to the 1 % solution is reported (no further information)
Source: Bayer AG Leverkusen
19-JAN-1996 (54)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method: other
Year: GLP: no data
Test substance: other TS: 1% in petrolatum
Remark: 0/17 thiuram sensitized patients had a positive patch test result with MBTS
Source: Bayer AG Leverkusen
22-JAN-1996 (55)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method: other
Year: GLP: no data
Test substance: other TS: 1% in petrolatum
Remark: 2/3 patients with allergic contact dermatitis from rubber footwear had a positive patch test result with MBTS
Source: Bayer AG Leverkusen
22-JAN-1996 (56)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP: no data
Test substance: other TS
Remark: result: 17 subjects allergic to mercaptobenzothiazole were found positive when tested with a 1 % solution (solvent unknown); tests were negative in 20 controls
Source: Bayer AG Leverkusen
13-MAY-1993 (57)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP: no data
Test substance: other TS
Remark: result: 3/13 persons were allergic to the upper material of safety shoes containing mercaptobenzothiazole or the disulfide; tests with the pure substances (1 %) were negative
Source: Bayer AG Leverkusen
13-MAY-1993 (58)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP: no data
Test substance: other TS
Remark: result: 5/21 persons who had a contact dermatitis when wearing certain kind of shoes were positive when tested with 1 % of the test substance in petrolatum; 4 of these 5 persons also reacted positive with mercaptobenzothiazole
Source: Bayer AG Leverkusen
13-MAY-1993 (59)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP: no data
Test substance: other TS: 5 % in petroleum or polyethylene glycol
Remark: result: an 8-year old boy with contact dermatitis against tennis shoes reacted positive when tested with the test substance or mercaptobenzothiazole
Source: Bayer AG Leverkusen
13-MAY-1993 (60)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP: no data
Test substance: other TS: 0.25 % solution in paraffine
Remark: 0/6 persons reacted positive when tested with "mercaptomix", which, among others, contained the test substance
Source: Bayer AG Leverkusen
13-MAY-1993 (61)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP: no data
Test substance: other TS
Remark: result: 50/78 men and 33/70 women were positive when tested with 1 % of the test substance (solvent unknown); in most cases a cross reaction with mercaptobenzothiazole was noted
Source: Bayer AG Leverkusen
13-MAY-1993 (62)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP: no data
Test substance: other TS
Remark: result: 25/1698 persons reacted positive when tested with 2 % of the test substance diluted in paraffin; cross reactions with other vulcanization accelerators were noted.
Source: Bayer AG Leverkusen
13-MAY-1993 (63)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP: no data
Test substance: no data
Remark: result: A miner with contact eczema had a positive patch test reaction with MBTS and MBT.
Source: Bayer AG Leverkusen
22-APR-1993 (64)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP: no data
Test substance: other TS: Vulkazite DM
Remark: result: 1/5 patients with contact dermatitis against rubber reacted positive (this patient reacted positive to other accelerators too)
Source: Bayer AG Leverkusen
22-APR-1993 (65)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP: no data
Test substance: other TS: 1 % in vaseline
Remark: result: 1/21 patients with contact dermatitis reacted positive
Source: Bayer AG Leverkusen
22-APR-1993 (66)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP: no data
Test substance: other TS: 1 % pet.
Remark: result: 0/15 thiuram-sensitized patients reacted positive
Source: Bayer AG Leverkusen
22-APR-1993 (55)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP: no data
Test substance: no data
Remark: method: no data
result: 10/21 contact dermatitis patients against rubber showed a positive reaction (MBT was positive too)
Source: Bayer AG Leverkusen
22-APR-1993 (67)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle: Petrolatum
Result:
Classification:
Method:
Year: GLP:
Test substance: other TS: purity: 1 % in pet.
Result: 0/9 patients with contact dermatitis due to rubber boots reacted positive
Source: Bayer AG Leverkusen
04-NOV-1998 (68)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle: Petrolatum
Result:
Classification:
Method:
Year: GLP:
Test substance: other TS: 1 % in pet.
Remark: 1/11 patients with allergic patch test reactions caused by cyclohexyl thiophthalimide showed a positive reaction with MBTS
Source: Bayer AG Leverkusen
04-NOV-1998 (69)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle: Petrolatum
Result:
Classification:
Method:
Year: GLP:
Test substance:
Remark: A 45-year-old contact dermatitis patient due to a rubber disc reacted positive with MBTS among each other.
Source: Bayer AG Leverkusen
04-NOV-1998 (70)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle: Petrolatum
Result:
Classification:
Method:
Year: GLP:
Test substance: other TS: 1 % in pet.
Remark: 0/5 patients with allergic contact dermatitis caused by thiourea compounds showed a positive reaction with MBTS
Source: Bayer AG Leverkusen
04-NOV-1998 (71)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP:
Test substance:
Remark: 309/317 (1.9 %) patients tested with the rubber tray had a positive response to MBTS. 22 % had a positive response to at least 1 of the allergens on the rubber tray.
Source: Bayer AG Leverkusen
04-NOV-1998 (72)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle: other: vaseline
Result:
Classification:
Method:
Year: GLP:
Test substance: other TS: 0.5 % in vas.
Remark: 3/135 patients with skin problems due to rubber chemicals showed a positive allergic reaction with MBT
Source: Bayer AG Leverkusen
04-NOV-1998 (73)

Type: Patch-Test
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP:
Test substance:
Remark: 30/53 patients with an allergic reaction to the Mercapto Mix showed a positive reaction with MBTS
Source: Bayer AG Leverkusen
04-NOV-1998 (74)

Type:	other: see remarks
Species:	human
Number of Animals:	
Vehicle:	
Result:	
Classification:	
Method:	other: see remarks
Year:	GLP: no data
Test substance:	other TS: 70 % preparation in petrolatum
Remark:	method: repeated insult patch test; a series of 12 applications (each of 24 h duration) of 0.2 g on the back of 53 persons was done through weeks 1-3, during week 6 a series of 4 applications (each of 24 h duration) of 0.2 g was done on virgin sites result: according to authors: not sensitizing
Source:	Bayer AG Leverkusen

13-MAY-1993 (47)

5.4 Repeated Dose Toxicity

Species:	rat Sex: no data
Strain:	no data
Route of admin.:	oral feed
Exposure period:	31 days
Frequency of treatment:	continuously in diet
Post. obs. period:	no data
Doses:	5000, 10000 or 20000 ppm (approx. 375, 750 or 1500 mg/kg bw/d)
Control Group:	no data specified
Method:	other
Year:	GLP: no data
Test substance:	no data
Result:	growth retardation, no pathological changes (no further details available)
Source:	Bayer AG Leverkusen

13-MAY-1993 (38)

Species: rat Sex: female
Strain: Wistar
Route of admin.: oral feed
Exposure period: 1st-21st day of gestation
Frequency of treatment: daily
Post. obs. period: yes
Doses: 0.04; 0.2; 1 % in diet (approx. 26, 127, 596 mg/kg/d)
Control Group: yes
NOAEL: 127 mg/kg
Method: other
Year: GLP: no data
Test substance: no data
Remark: see also chapter 5.8
Result: 596 mg/kg: weight reduction until 15th day of gestation
Source: Bayer AG Leverkusen
13-MAY-1993 (75)

Species: rat Sex: male
Strain: other: Wistar Albino
Route of admin.: gavage
Exposure period: 10 days
Frequency of treatment: daily
Post. obs. period: no data
Doses: 400 or 800 mg/kg bw/d
Control Group: no data specified
Method: other
Year: GLP: no data
Test substance: no data
Remark: oil suspension
no further information available
Result: 400 mg/kg: reduced concentrations of total and reduced glutathione in blood, reduced activity of AP-enzyme in serum (78 %) and GPT-enzyme in liver (90 %) and kidneys (80 %); changes of cell proteins in liver and kidneys
800 mg/kg: reduced concentrations of total and reduced glutathione in blood, reduced activity of AP-enzyme in serum (70 %) and GPT-enzyme in liver (90 %) and kidneys (58,5 %); no information about cell proteins; unchanged weights of liver, kidneys, mill and supra-renal glands.
Source: Bayer AG Leverkusen
13-MAY-1993 (39)

Species: rat Sex: male/female
Strain: other: Albino
Route of admin.: gavage
Exposure period: females: before pregnancy on the 1st and 3rd day of estrus
males: same time as females, but twice within 3 days
Frequency of treatment: see above
Post. obs. period: until 19th day of pregnancy
Doses: 200 mg/kg bw/d
Control Group: yes
Method: other: "pseudo dominant-lethal-test" (11 females, number of males not noted; in sunflower oil)
Year: GLP: no data
Test substance: no data
Remark: see also chapter 5.8
Result: females: no visible signs of poisoning
males: no data
Source: Bayer AG Leverkusen
13-MAY-1993 (76)

Species: rat Sex: female
Strain: Wistar
Route of admin.: gavage
Exposure period: whole gestation
Frequency of treatment: daily
Post. obs. period: no data
Doses: 10 or 100 mg/kg bw/d
Control Group: yes
Method: other
Year: GLP: no data
Test substance: no data
Remark: method: 60 animals tested; suspension in sunflower oil
remarks: no further information available
Result: 100 mg/kg: increased activity of glutamatoxalacetattrans-aminase (up to 116%) and glutamatpyruvattransaminase (up to 101%) on day 21, decreased activity of the liver enzymes
10 mg/kg: similar effects like 100 mg/kg, statistically not significant
Source: Bayer AG Leverkusen
13-MAY-1993 (77)

Species: rat Sex: female
Strain: Wistar
Route of admin.: gavage
Exposure period: 3 months
Frequency of treatment: daily
Post. obs. period: no data
Doses: 100 mg/kg bw/d
Control Group: yes
Method: other
Year: GLP: no data
Test substance: no data
Remark: method: 40 animals tested
remarks: no further information available
Result: no clinical signs of intoxication; inhibition of lactate- and malate-dehydrogenase activity
Source: Bayer AG Leverkusen
13-MAY-1993 (77)

Species: mouse Sex: male/female
Strain: other: C57BL/6xC3h/Anf, C57BL/6xAKR (both F1-hybrides)
Route of admin.: other
Exposure period: 3 weeks with stomach tube followed by 17 months in diet
Frequency of treatment: daily
Post. obs. period: no
Doses: 464 mg/kg bw/d (stomach tube); approx. 237 mg/kg bw/d (in diet)
Control Group: yes
Method: other
Year: GLP: no data
Test substance: no data
Remark: the maximal tolerated doses were given;
original data: 1577 ppm in diet
see also chapter 5.7
Result: no significant effects on organs observed during external and histologic examinations of major organs (no further information)
Source: Bayer AG Leverkusen
11-APR-1995 (78)

Species: guinea pig Sex: no data
Strain: no data
Route of admin.: inhalation
Exposure period: 6 days
Frequency of treatment: 1 hour/day
Post. obs. period: no data
Doses: 0.1 mg/l
Control Group: no data specified
Method: other
Year: GLP: no data
Test substance: no data
Remark: exposure to 2,2'-dithiobisbenzothiazole-dust; concentration (no data whether analytical or nominal): 100 mg/m3; no further information available
Result: no mortality; histopathological changes in liver (fatty tissue) and kidneys; pneumonia and bronchitis
Source: Bayer AG Leverkusen
13-MAY-1993 (40)

Species: guinea pig Sex: no data
Strain: no data
Route of admin.: oral unspecified
Exposure period: no data
Frequency of treatment: 5 times
Post. obs. period: no data
Doses: 0.5 or 1 g/kg bw
Control Group: no data specified
Method: other
Year: GLP: no data
Test substance: no data
Remark: no further information available
Result: 0.5 g/kg: no symptoms were observed
1 g/kg: 1/5 animals died after 76 h, the others showed reduced mobility and extreme indolence within 48 h, fatty tissue in the liver and granulated degeneration of the renal channel epithel
Source: Bayer AG Leverkusen
13-MAY-1993 (40)

5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537
Concentration: <= 0.1 mg/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: GLP: no data
Test substance: no data
Source: Bayer AG Leverkusen
13-MAY-1993 (79)

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100
Concentration: <= 0.1 mg/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result:
Method: other
Year: GLP: no data
Test substance: no data
Remark: result: negative without S9 mix
weakly positive with S9 mix
Source: Bayer AG Leverkusen
13-MAY-1993 (80)

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration: <= 5 mg/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: GLP: no data
Test substance: no data
Source: Bayer AG Leverkusen
13-MAY-1993 (81)

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100
Concentration: <= 1 mg/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: GLP: no data
Test substance: no data
Remark: also negative result after in vitro nitrosation
Source: Bayer AG Leverkusen
13-MAY-1993 (82)

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537
Concentration: <= 1 mg/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: GLP: no data
Test substance: other TS: purity 95 %
Source: Bayer AG Leverkusen
13-MAY-1993 (83) (84)

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration: no data
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: GLP: no data
Test substance: no data
Source: Bayer AG Leverkusen
13-MAY-1993 (85) (86)

Type: Ames test
System of testing: Salmonella typhimurium TA 97, TA 98, TA 100, TA 1535
Concentration: <= 10 mg/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: positive
Method: other
Year: GLP: no data
Test substance: no data
Source: Bayer AG Leverkusen
13-MAY-1993 (87)

Type: Ames test
System of testing: Salmonella typhimurium TA 97, TA 98, TA 100, TA 102
Concentration: <= 10 mg/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: GLP: no data
Test substance: no data
Source: Bayer AG Leverkusen
13-MAY-1993 (88)

Type: Ames test
System of testing: Salmonella typhimurium TA 97, TA 98, TA 100, TA 1535, TA 1538
Concentration: <= 1.0 mg/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: 1982 GLP: yes
Test substance: other TS: no data
Remark: GLP: Signed Quality Unit Audit Statement
Source: Bayer AG Leverkusen
19-APR-1994 (89)

Type: Ames test
System of testing: Salmonella typhimurium
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:
Test substance: other TS: MBTS purity = 98%
26-APR-2001 (90) (91)

Type: Bacterial gene mutation assay
System of testing: Escherichia coli WP2uvrA-
Concentration: <= 5 mg/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: modified Ames test
Year: GLP: no data
Test substance: other TS: 80 % purity
Source: Bayer AG Leverkusen
13-MAY-1993 (81)

Type: Cytogenetic assay
System of testing: Chinese hamster ovary cells
Concentration: <= 10 mg/l
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other
Year: GLP: no data
Test substance: other TS: 80 % purity
Source: Bayer AG Leverkusen
13-MAY-1993 (81)

Type: DNA damage and repair assay
System of testing: Escherichia coli W3110 (pol A+) and p3078 (pol A-)
Concentration: <= 5 mg/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: ambiguous
Method: other
Year: GLP: no data
Test substance: other TS: 80 % purity
Remark: solubility prevents obtaining toxic dose in plate assay
Source: Bayer AG Leverkusen
13-MAY-1993 (81)

Type: Gene mutation in Saccharomyces cerevisiae
System of testing:
Concentration:
Cytotoxic Conc.:
Metabolic activation: no data
Result: negative
Method:
Year: GLP:
Test substance:
Source: Monsanto
Bayer AG Leverkusen
10-MAY-1994 (92)

Type: HGPRT assay
System of testing: CHO cells
Concentration: 1.25 - 80 ug/ml
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: no data
Year: GLP: no data
Test substance: other TS: as prescribed by chapter 1 in dataset of ELF ATOCHEM
Remark: Year: 1982-1984
Source: ELF ATOCHEM S.A., France
Bayer AG Leverkusen
10-MAY-1994 (93)

Type: HGPRT assay
System of testing: CHO cells
Concentration: 25 - 1500 ug/ml
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: no data
Year: 1986 GLP: no data
Test substance: other TS: as prescibed by chapter 1 in dataset of ELF ATOCHEM
Source: ELF ATOCHEM S.A., France
Bayer AG Leverkusen
10-MAY-1994 (93)

Type: Mouse lymphoma assay
System of testing: mouse lymphoma cell line L5178Y TK+/-
Concentration: <= 30 mg/l
Cytotoxic Conc.:
Metabolic activation: with and without
Result:
Method: other
Year: GLP: no data
Test substance: other TS: 80 % purity
Remark: result: negative without S9 mix
positive with S9 mix (lowest active dose: 0.015 mg/ml)
Source: Bayer AG Leverkusen
13-MAY-1993 (81)

Type: Mouse lymphoma assay
System of testing: mouse lymphoma cells (no further information)
Concentration: no data
Cytotoxic Conc.:
Metabolic activation: no data
Result: negative
Method:
Year: GLP: no data
Test substance: other TS: purity = 98%
Source: Bayer AG Leverkusen
26-APR-2001 (94)

Type: Mouse lymphoma assay
System of testing: L5178Y cells
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP: no data
Test substance: other TS: MBTS purity = 98%
Remark: MBTS did not significantly induce mutations in the lk locus with or without metabolic activitation
Source: Monsanto
Bayer AG Leverkusen
06-NOV-2000 (95)

Type:
System of testing: Salmonella
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:
Test substance: other TS: trapped effluent samples containing phr MBTS
Source: Monsanto
Bayer AG Leverkusen
26-APR-2001 (96) (97)

5.6 Genetic Toxicity 'in Vivo'

Type: other
Species: Sex: male/female
Strain:
Route of admin.: oral unspecified
Exposure period: twice within 3 days (m); 1st 3rd day of oestrus
Doses: 200 mg/kg
Result:
Method: other
Year: GLP: no data
Test substance: other TS: Altax
Remark: Unsuitable test system (e.g. treatment of both sexes)
Result: Increased postimplantation embryonic mortality (= "index of mutagenicity")
Source: Bayer AG Leverkusen
23-JAN-1996 (76)

5.7 Carcinogenicity

Species: mouse Sex: male/female
Strain: other: C57BL/6xC3h/Anf, C57BL/6xAKR (both F1-hybrides)
Route of admin.: other
Exposure period: 3 weeks with stomach tube followed by 17 months in diet
Frequency of treatment: daily
Post. obs. period: no
Doses: 464 mg/kg bw/d (stomach tube), approx. 237 mg/kg bw/d (in diet)
Result:
Control Group: yes
Method: other
Year: GLP: no data
Test substance: no data
Remark: number of animals: 18 of each sex of each strain
necropsy: external examination with histologic examination of major organs and of all grossly visible lesions

(no further information)
strains: C57BL/6xC3h/Anf, C57BL/6xAKR (both F1-hybrides)
original data: 1577 ppm in diet
see also chapter 5.4.
Result: no significant increase of tumors
Source: Bayer AG Leverkusen
11-APR-1995 (78)

Species: mouse Sex: male/female
Strain: other: B6C3F1, B6AKF1
Route of admin.: s.c.
Exposure period: once on 18th day of life
Frequency of treatment:
Post. obs. period: 18 months
Doses: 1000 mg/kg
Result:
Control Group: yes
Method: other
Year: GLP: no data
Test substance: no data
Remark: method: 18 animals/sex tested; in gelatine
remarks: strains: B6C3F1, B6AKF1
Result: The tumor rate was not increased significantly compared to control animals (0.5 % gelatine)
Source: Bayer AG Leverkusen
13-MAY-1993 (98)

Species: other: (see method) Sex:
Strain:
Route of admin.:
Exposure period:
Frequency of treatment:
Post. obs. period:
Doses:
Result:
Control Group:
Method: other: celltransformation test with BALB/3T3 cells according to Kakunaga, T., Int. J. Cancer 12, 463-473 (1973); in DMSO
Year: GLP: no data
Test substance: other TS: 80 % purity
Remark: result: number of foci not increased
Source: Bayer AG Leverkusen
22-APR-1993 (81)

5.8 Toxicity to Reproduction

Type: other
Species: rat Sex: male/female
Strain: other: Albino
Route of admin.: gavage
Exposure Period: females: before pregnacy, on the 1st and 3rd day of estrus - males: at the same time as females, twice within 3 days
Frequency of treatment: see above
Duration of test: sacrifice on day 19
Doses: 200 mg/kg bw
Control Group: yes
Method: other
Year: GLP: no data
Test substance: no data
Remark: unsuitable test system (e.g. number of males not noted; treatment of both sexes)
Result: dams: no visible signs of poisoning; changes in the estrus cycle, often no conception in the next cycle, greatest retardation of cycle: 6.9+/-0.9 days
offspring: decreased body weight, decreased fertility (46 %), increased embryo mortality (56.4+/-3.8 %; controls: 10.9+/-1.6 %), increased postimplantation loss (30.8+/-4.4 %; controls: 4.6+/-1.1 %)
Source: Bayer AG Leverkusen
23-JAN-1996 (76)

Type: other: (see method)
Species: Sex:
Strain:
Route of admin.:
Exposure Period:
Frequency of treatment:
Duration of test:
Doses:
Control Group:
Method: other: test substance was tested for embryotoxicity and induction of malformations in three-day chicken embryos (application: injection into the air bubble of the egg or into the heart); in acetone
Year: GLP: no data
Test substance: no data
Remark: result: no effects were observed
Source: Bayer AG Leverkusen
22-APR-1993 (99) (100)

5.9 Developmental Toxicity/Teratogenicity

Species: rat Sex: female
Strain: other: Albino
Route of admin.: gavage
Exposure period: 8 days
Frequency of treatment: on day 4 and 11 of gestation
Duration of test: sacrifice on day 19
Doses: 200 mg/kg bw
Control Group: yes
Method: other
Year: GLP: no data
Test substance: no data
Remark: method: 15 animals tested; in corn oil
Result: Foetal data: decreased weight of fetuses; increase of total embryo mortality (37.8+/-3.2 %; controls:10.9+/-1.6%); Maternal general toxicity:lengthening of oestrus cycle and reduced fertility (30 %); increased postimplantation loss (15.4+/-2.7%; controls: 4.6+/-1.1 %)
Source: Bayer AG Leverkusen
06-NOV-2000 (76)

Species: rat Sex: female
Strain: Wistar
Route of admin.: gavage
Exposure period: whole gestation
Frequency of treatment: daily
Duration of test:
Doses: 10 or 100 mg/kg bw
Control Group: yes
Method: other
Year: GLP: no data
Test substance: no data
Remark: method: 30 animals/dose; in grease
Result: 10 mg/kg: no embryotoxic effects
100 mg/kg: no embryotoxic effects, changes in enzyme activities of liver and blood, increased relative organ weights of liver and kidneys, reduced RNA in liver cells, slightly dystrophic alterations in placentae
Source: Bayer AG Leverkusen
13-MAY-1993 (101)

Species: rat Sex: female
Strain: Wistar
Route of admin.: oral feed
Exposure period: 1st-21st day of gestation
Frequency of treatment: daily
Duration of test: see remarks
Doses: 0.04; 0.2; 1 % in diet (approx. 26, 127, 596 mg/kg/d)
Control Group: yes
NOAEL Maternalt.: .2 %
NOAEL Teratogen.: 1 %
Method: other
Year: GLP: no data
Test substance: no data
Remark: method: no data
NOEL (parenteral): 127 mg/kg bw
NOEL (offspring): 596 mg/kg
remarks:
follow-up period:
I. sacrifice of dams on day 21 of gestation
II. sacrifice of dams on day 21 after birth and offspring <= 7 weeks after birth
Result: 26, 127 mg/kg: no teratogenic effects;
596 mg/kg: weight reduction of dams until 15th day of gestation; no teratogenic effects
Source: Bayer AG Leverkusen
06-NOV-2000 (75)

Species: rat Sex: female
Strain: other: Wistar, Hybrid
Route of admin.: oral unspecified
Exposure period: 1st-21st, 1st-7th, 8th-12th or 13th-17th day of gestation
Frequency of treatment: daily
Duration of test:
Doses: 10 or 100 mg/kg bw/d
Control Group: yes
NOAEL Teratogen.: 10 mg/kg bw
Method:
Year: GLP: no data
Test substance: no data
Remark: method: 120 animals tested; in water solution
NOEL (parenteral): no data
NOEL (offspring): 10 mg/kg
Result: 10 mg/kg: no embryotoxic effects
100 mg/kg:
1st-21st day of gestation: increased mortality of embryos, increased frequency of autolysis, reduced weight of embryos, changes of cranium dimensions, internal hydrocephalus, intracerebral hematoma, isolated hematoma (54.5%);
13th-17th day of gestation: increased mortality of embryos, increased frequency of autolysis, reduced weight of embryos, anormal ossification of the brain;
1st-7th and 8th-12th day of gestation: anormal ossification

of the brain
Source: Bayer AG Leverkusen
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
26-APR-2001 (102)

Species: mouse Sex: female
Strain: other: N strain
Route of admin.: oral unspecified
Exposure period: whole gestation
Frequency of treatment: daily
Duration of test: sacrifice at the end of gestation
Doses: 10 or 100 mg/kg
Control Group: yes
NOAEL Teratogen.: 10 mg/kg bw
Method: other
Year: GLP: no data
Test substance: no data
Remark: method: 40 animals tested; in water solution
NOEL (offspring): 10 mg/kg
Result: 10 mg/kg: no embryotoxic or teratogenic effects
100 mg/kg: no embryotoxic effects;
teratogenic effects: exencephalia, hypognatia, edema (5.5%; control: no data), hydrocephalia (72.7%; control: 33.3%), microphtalmia (9.1%; control: 4.8%).
Source: Bayer AG Leverkusen
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
26-APR-2001 (102)

5.10 Other Relevant Information

Type: Biochemical or cellular interactions
Remark: test substance: no data
remark: The results of in vitro experiments show that MBT is the only stable compound of different mercaptobenzo-thiazoles (e.g. MBTS) when reducing sulfhydryl compounds are present; these findings may explain the cross-sensitivities reported for the mercaptobenzothiazoles.
Source: Bayer AG Leverkusen
22-APR-1993 (103)

Type: other
Remark: revision: 10/98
Source: Bayer AG Leverkusen
04-NOV-1998

Type: other: effects on blood sugar
Remark: test substance: no data
effects: 100 mg/kg i.p. in physiological sodium chloride solution tended to increase blood sugar of 3 rabbits which had alloxan derived diabetes
Source: Bayer AG Leverkusen
22-APR-1993 (104)

Type: other: enzyme activity
Remark: test substance: no data
effects: 33.25 mg/kg given by stomach tube to female rats increased the benzpyrene hydroxylase activity in the liver after 48 h (1.5 fold in comparison with controls), but not in the lung
Source: Bayer AG Leverkusen
04-NOV-1998 (105)

Type: other: enzyme activity
Remark: test substance: no data
effects: < 2.33 mg/l in vitro did not have an activation effect on the carbohydrate metabolism of Ehrlich Ascites tumor cells
Source: Bayer AG Leverkusen
22-APR-1993 (106)

Type: other: metabolism/pharmacokinetics
Remark: test substance: purity of unlabeled test substance 94-99.4%; radiochemical purity 94.1-100%
effects: F 344 rats (4m/4f) were dosed by gavage with 0.547 mg/kg bw/d in corn oil for 14 d. Then they received a single oral dose of 0.73 mg/kg bw of the 14C-labeled test substance. After 96 h 60.8% (m) or 81.7% (f) of the radioactivity were found in urine and 8.6% (m) or 3.5% (f) in the feces, indicating that the test substance is well absorbed from the gastro-intestinal tract.
8 h after application of the labeled dose elevated levels of radioactivity were found in the thyroid glands and in the erythrocytes and kidneys; comparably low concentrations were found in the gonads and spleen. After 96 h tissue concentrations were generally low; the highest concentrations were in whole blood and thyroid.
Elimination half-life values (h) were as follows:

	alpha phase	beta phase
whole blood:	not discernable	239 (m), 3840 (f)
plasma:	4.32 (m), 3.91 (f)	102 (m), 138 (f)

Radioactivity excreted in the urine was confined to two polar metabolites being most probably a thioglucuronide and a sulfonic acid derivative of the monomer 2-mercaptobenzo-thiazole.
Source: Bayer AG Leverkusen
22-APR-1993 (107)

Type: other: metabolism/pharmacokinetics
Remark: test substance: purity of unlabeled test substance, as far as stated; analytical grade
effects: F 344 rats (4/dose/sex) were dosed by gavage with 0.438 or 51.1 mg/kg bw of the 14C-labeled test substance in corn oil. After 96 h most of the radioactivity was found in the urine (low dose: 95.8% (m), 82.9% (f); high dose: 94.3% (m), 90.7% (f)) and minor amounts in the feces (low dose: 7.27% (m), 4.91% (f); high dose: 10.3% (m), 4.94% (f)).
Elimination half-life values (h) were as follows:

	alpha phase	beta phase
low dose:		
whole blood:	7.63 (m), 4.58 (f)	7500 (m), 289 (f)
plasma:	4.32 (m), 3.91 (f)	102 (m), 138 (f)
high dose:		
whole blood:	6.39 (m), 8.03 (f)	25400 (m), 9610 (f)
plasma:	4.78 (m), 4.18 (f)	50200 (m), 6490 (f)

7 not identified metabolites were found in the urine.
Source: Bayer AG Leverkusen
22-APR-1993 (108)

Type: other: metabolism/pharmacokinetics
Remark: test substance: test substance contained 6-17% 2-mercapto-benzothiazole resulting from the peroxidizing activity of the solvent tetrahydrofuran.
effects: F 344 rats (4 animals/sex) were injected a single dose of the 14C-labeled test substance (0.571 mg/kg bw) into the tail vein. After 72 h most of the radio activity was found in the urine (92.9% (m), 101.9% (f)) and minor amounts in the feces (9.64% (m), 3.82% (f)).
Elimination half-life values (h) were as follows:

	alpha phase	beta phase
whole blood:	0.87 (m), 0.47 (f)	89.9 (m), 55.1(f)
plasma:	1.29 (m), 0.64 (f)	18.9 (m), 13.2 (f)

Source: Bayer AG Leverkusen
22-APR-1993 (107)

Type: other: metabolism/pharmacokinetics
Remark: test substance: purity of unlabeled test substance 94-99.4%; radiochemical purity: 94.1-100%
effects: 96 h after occlusive application of a single dose of the 14C-labeled test substance in tetrahydrofuran (0.034 mg/animal) on the scarified skin (area: 2 cmE2) of F 344 rats (4 animals/sex) 88.2% (m) resp. 92.8% (f) of the total absorbed dose were found in urine and 8.7% (m) resp. 5.3% (f) in the feces.
Elimination half-life values (h) were as follows:

	alpha phase	beta phase
whole blood:	0.87 (m), 0.47 (f)	89.9 (m), 55.1 (f)
plasma:	1.29 (m), 0.64 (f)	18.9 (m), 13.2 (f)

Source: Bayer AG Leverkusen
22-APR-1993 (107)

Type: other: metabolism/pharmacokinetics
Remark: test substance: purity of unlabeled test substance 94-99.4% radiochemical purity 94.1-100%.
effects: 96 h after occlusive application of a single dose of the 14C-labeled test substance in tetrahydrofuran (0.034 mg/animal) on the scarified skin (area: 5 cmE2) of 3 female guinea pigs (Hartley) 96.7% of the total absorbed dose were found in the urine and 2.3% in the feces.
Source: Bayer AG Leverkusen
22-APR-1993 (107)

Type: other: metabolism/pharmacokinetics
Remark: After a single dose of 25 mg 14C-MBTS/rat over 90% of the S atoms of urinary metabolites were derived from the parent compound (no detailed information on the metabolites). Excretion predominately into faeces (71.9% radioactivity).
Source: Bayer AG Leverkusen
23-JAN-1996 (109)

Type: other: metabolism/pharmacokinetics
Remark: A single oral dose of 125 mg 14C-MBTS/kg (3m): ca. 21% radioactivity in urine and 72% in faeces (total recovery after 3 days = 93%)
Single injection of 14C-MBTS into the jejunal loop: The radioactivity absorbed was ca. 6.4% shared between MBT and MBTS with a ratio of 1:3 in the plasma.
Incubation with rat liver/kidney homogenate: Transformation to MBT and its glucoronide and sulfate.
Source: Bayer AG Leverkusen
24-JAN-1996 (110)

5.11 Experience with Human Exposure

Remark: In a repeat insult patch test conducted with 53 human volunteers, MBTS did not demonstrate that it was a primary or a cummulative irritant or a skin sensitizer.
Source: Monsanto
Bayer AG Leverkusen
10-MAY-1994 (111)

(1) Windholz, M., The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals, 10th ed. Rahway, New York, 492-493 (1983)

(2) Keith, L.H. & Walters, D.B., Compendium of Safety Data Sheets for Research and Industrial Chemicals, VCH, Verlagsgesellschaft mbH, Weinheim, 2462-2465 (1987)

(3) Bayer data, DIN-Sicherheitsdatenblatt Dibenzothiazyldisulfid (MBTS), Bayer AG, Leverkusen (1988)

(4) Monsanto data

(5) Boberg, M. et al., Thiazole und Isothiazole; Benzothiazole, cited in: Ullmanns Enzyklopaedie der technischen Chemie, 4. Aufl., Bd. 23, Verlag Chemie, 143-151 (1983)

(6) Merck Index (1989)

(7) Kempermann, T. & Eholzer, U., Bayer AG, Leverkusen, T.I.B. Kautschuk-Chemikalien, Nr. 1.8., 8 pp. (1983)

(8) Bayer AG data

(9) Monsanto Studies SR-83X-64 and SR-85-X017

(10) SRI International, Project No. 8669 from 20.8.1980

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

(12) SRI International, Project No. 8669 from 20.8.1990

(13) Monsanto SR-83-64, SR 85-017 SRI International, 1983 and 1985.

(14) Biodegradation and Bioaccumulation Data of Existing Chemicals Based on the CSCL Japan, Compiled under the Supervision of Chemical Products Safety Division, Basic Industries Bureau MITI, Ed. by CITI, October 1992. Published by Japan Chemical Industry Ecology-Toxicology & Information Center

(15) Monsanto Studies SR-83X-64 and SR-85-X017 (1983 and 1985)

(16) Behnke, W., Berechnung nach Atkinson zum photochemischen Abbau in der Athmosphaere. Unveroeffentlichte Berechnung, Fraunhofer-Institut fuer Toxikologie und Aerosolfoschung, Abt. Physikalische Chemie, Hannover (1990)

(17) Abdou, W.M. et al., Z. Naturforsch. 42b, 1153-1158 (1987)

(18) Monsanto Study AB-84X-129 (ES-80-SS-42), Analytic Bio-Chemistry Lab, 1984

(19) Monsanto Co. data, NTIS OTS0206761, EPA OTS document

(20) Environmental Agency Japan, Background paper on the experience of the environmental monitoring of chemical substances in Japan. Proceedings of the workshop on the control of existing chemicals under the patronage of the OECD. Umweltbehoerde Japan, Umweltbundesamt Berlin, 165 - 189 (1981)

(21) Bosch et al., Technical support document 2-Mercaptobenzthiazoles (SRC-TR-85-104; Contract No. 68-02-4209). Syracuse Research Corporation, Syracuse, New York (1985)

(22) Monsanto Study BN-76-170, EG&G Bionomics (1976)

(23) Monsanto Study BN-79-219, EG&G Bionomics (1979)

(24) Monsanto Study BN-76-170

(25) Monsanto Study SR-83X-64 and SR-85-X017

(26) Monsanto Study BN-79-220, EG&G Bionomics (1979)

(27) Monsanto Study BN-79-218, EG&G Bionomics (1979)

(28) Tomlinson, T.G. et al., J. Appl. Bact. 29, 266-291 (1966)

(29) Suzuki, S. & Nakajima, T., Kogyo Yosui 103, 50-53 (1967)

(30) Williams, G.R., Int. Biodeterior. 20, 173-175 (1984)

(31) Bounaga, N., Phytopath. Z. 98, 210-217 (1980)

(32) Younger Laboratories, Monsanto Co., St. Louis, Missouri (1973); Monsanto Study Y-73-190

(33) Vanderbilt data, Material Safety Data Sheet for Benzothiazyl Disulfide, R.T. Vanderbilt Co., Inc., Norwalk, Connecticut (1990)

(34) Food Preserves Hygiene Council Reports No. 22, 17 (1973); cited in: Takahashi, A., Int. Polym. Sci. Techn. 3, 93-105 (1976)

(35) Vaisman, Y.I. et al., Gig. Sanit. 30, 17-21 (1973)

(36) Vernot, E.H. et al., Toxicol. Appl. Pharmacol. 42, 417-423 (1977)

(37) Sumitomo data, Acute oral toxicity of Soxinol DM in rats, Sumitomo Chemical Co. LTD., report No. PDT-No. C-77-114 (1977)

(38) Amer. Cyan. Co.; cited in: McCormick, W.E., Rubber Chem. Technol. 44, 512-533 (1971)

(39) Radeva, M., Chig. Chran. 23, 326-330 (1980) (in Bulgarisch; dtsch. Kurzuebersetzung)

(40) Kowalski, Z. & Bassendowska, E., Medycina Pracy 16, 35-43 (1965) (in Polnisch; dtsch. Kurzuebersetzung)

(41) Younger Laboratories, Monsanto Co., St. Louis, Missouri (1973); Monsanto Study Y-73-190 and Y-72-327

(42) Doull, J. et al., Armed Services Technical Information Agency, Arlington, Virginia, NTIS-Publication No. AD 277-689 (1962)

(43) US Army data; cited in: RTECS data base (1992)

(44) Younger Laboratories, Monsanto Co., St. Louis, Missouri (1973) Study# Y-73-190

(45) Monsanto Study Y-73-190

(46) IG Farben, Mitteilung des Gewerbehygienischen I. G. Labors vom 30.7.31 (unpublished). Ludwigshafen (1931)

(47) Monsanto data, Monsanto Company, St. Louis, Missouri, report No. PI 2600, 30 pp. (1982)

(48) Younger Laboratories, Monsanto Co., St. Louis, Missouri (1973)

(49) Nakamura, A. et al., Contact Dermatitis 31, 72-85 (1994)

(50) Kaniwa, M.-A. et al., Contact Dermatitis 27, 166-173 (1992)

(51) Kiec-Swierczynska, Contact Dermatitis 32, 171-172 (1995)

(52) Bandmann, H.J. & Nasemann, Th., Der Hautarzt 9, 40-41 (1958)

(53) Conde-Salazar, L. et al., Journal of the American Academy of Dermatology 29, 176-180 (1993)

(54) Emmet, E.A. et al., Contact Dermatitis 30, 85-90 (1994)

(55) Knudsen, B.B. et al., Contact Dermatitis 28, 63-69 (1993)

(56) Kaniwa, M.-A. et al., Contact Dermatitis 30, 26-34 (1994)

(57) Foussereau, J. et al., Contact Dermat. 9, 514-516 (1983)

(58) Foussereau, J. et al., Contact Dermat. 14, 233-236 (1986)

(59) Blank, I.H. & Miller, O.G., J. Am. Med. Assoc. 149, 1371-1374 (1952)

(60) Jung, J.H. et al., Contact Dermat. 19, 254-259 (1988)

(61) Te Lintum, J.C.A. & Nater, J.P., Berufsdermatosen 21, 16-22 (1973)

(62) Cronin, E., Churchill Livingstone, Edinburgh, London, New York, 915 pp. (1980)

(63) Rudzki, E. et al., Contact Dermatitis 2, 24-27 (1976)

(64) Hegyi, E. Prac. Lek. 42 (10), 436-437 (1990)

(65) Bandmann, H.-J., Hautarzt 7, 419-421 (1956)

(66) Frosch, P.J. et al., Hautarzt 38, 210-217 (1987)

(67) Schultheiss, E., Berufsdermatosen 7, 76-97 (1959)

(68) Nishioka, K. et al., Contact Dermatitis 35, 241-245 (1996)

(69) Kanerva, L. et al., Contact Dermatitis 34, 23-26 (1996)

(70) Mitxelena, J. et al., Contact Dermatitis 38, 181-182 (1998)

(71) Kanerva, L. et al., Contact Dermatitis 31, 242-248 (1994)

(72) Holness, D.L. & Nethercott, J.R., Contact Dermatitis 36, 207-211 (1997)

(73) Heise, H. et al., Dermatosen 45, 226-228 (1997)

(74) Geier, J. & Gefeller, O., Am. J. Contact Dermatitis 6, 143-149 (1995)

(75) Ema, M. et al., J. Appl. Toxicol. 9, 413-417 (1989)

(76) Aleksandrov, S.E., Byull. Eks. Biol. Med. 93, 87-88 (1982) (in Russisch; engl. Uebersetzung)

(77) Mirkova, E., Chig. Zdraveop. 23, 414-419 (1980) (in Bulgarisch; dtsch. Kurzuebersetzung)

(78) Innes, J.R.M. et al., J. Nat. Cancer Inst. 42, 1101-1114 (1969)

(79) Goodyear data, laboratory report No. 79-58, Akron., Ohio, November 8 (1979)

(80) You, X. et al., Huanjing Kexue 3, 39-42 (1982) (in Chinesisch; dtsch. Uebersetzung)

(81) Hinderer, R.K. et al., Environ. Mutagenesis 5, 193-215 (1983)

(82) Crebelli, R. et al., Toxicol. Lett. 23, 307-313 (1984)

(83) Crebelli, R. et al., Brit. J. Ind. Med. 42, 481-487 (1985)

(84) Crebelli, R. et al., IARC Sci. Publ. 59, 289-295 (1984)

(85) Donner, M. et al., Scand. J. Work Environ. Health 9, 27-37 (1983)

(86) Rannug, A. et al., Prog. Clin. Biol. Res. 141, 407-419 (1984)

(87) Zeiger, E., Environ. Mol. Mutagen. 11, Suppl. 12, 1-158 (1988)

(88) Hinderer, R.K., Ames Salmonella Microsome, BFG Quality Assurance Unit (1984)

(89) The BF Goodrich Company data, 12-15-1982, Laboratory Identification Number 14

(90) Industrial Hazards of Plastics & Synthetic Elastomers (1984)

(91) Monsanto BO-76-178, Litton Bionetics (1976)

(92) Monsanto Study BO-76-178

(93) ELF ATOCHEM, Synopsis of Mutagenicity Data, 2-Mercaptobenzothiazole disulfide, August 1986

(94) Monsanto data (1982); cited in: Bosch, S.J. et al., Technical Support Document: 2-Mercaptobenzothiazoles. Syracuse Research Corporation, New York (1985)

(95) Monsanto Study BO-78-239, Litton Bionetics (1978)

(96) Monsanto Study ML-79-39

(97) Monsanto Study ML-79-44

(98) NCI, Public Health Service Publication No. 149, National Cancer Institute, Washington, D.C., Government Printing Office (1968), cited in: Holleman, J., Chemical Hazard Information Profile (Draft Report): Mercaptobenzothiazole disulfide (MBTS) (CAS-No. 120-78-5). Chemical Effects Information Center, Oak Ridge National Laboratory, 32 pp (1983).

(99) Korhonen, A. et al., Arch. Environ. Contam. Toxicol. 11, 735-759 (1982)

(100) Korhonen, A. et al., Scand. J. Work Environ. Health 9, 115-119 (1983)

(101) Radeva, M. & Dinoeva, S., Chig. Zdraveop. 26, 51-55 (1983) (in Bulgarisch; dtsch. Kurzuebersetzung)

(102) Mirkova, E., Probl. Higien. 5, 83-91 (1980) (in Russisch; engl. Uebersetzung)

(103) Hansson, C. and Agrup, G., Contact Dermatitis 28, 29-34 (1993)

(104) Chiba, T., Yakugaku Zasshi 89, 1138-1143 (1969) (in Japanisch; dtsch. Kurzuebersetzung)

(105) Wattenberg, L.W. et al., Cancer Res. 28, 2539-2544 (1968)

(106) Grassetti, D.R. et al., J. Med. Chem. 13, 273-276 (1970)

(107) El Dareer, S.M. et al., J. Toxicol. Environ. Health 27, 65-84 (1989)

(108) Hill, D.L., Disposition of 2-mercaptobenzothiazole-ring-UL-14C and 2-mercaptobenzothiazole disulfide-ring-UL-14C in Fischer-344 male and female rats dosed orally. Southern Research Institute, Birmingham, Alabama, 46 pp. (Report 5873-I) (1986)

(109) Fukuoka, M. & Tanaka, A., Arch. Toxicol. 61, 158-160 (1987)

(110) Fukuoka, M. et al., Arch. Toxicol. 70, 1-9 (1995)

(111) Monsanto Study SH-82-9

7.1 End Point Summary

-

7.2 Hazard Summary

-

7.3 Risk Assessment

-