

201-14999B

I U C L I D

Data Set

RECEIVED
OPPT 0910
04 JAN - 6 PM 1:26

Existing Chemical : ID: 2231-57-4
CAS No. : 2231-57-4
EINECS Name : thiocarbonohydrazide
EC No. : 218-769-8
Molecular Formula : CH6N4S

Producer related part

Company : Bayer Corporation
Creation date : 11.11.2003

Substance related part

Company : Bayer Corporation
Creation date : 11.11.2003

Status :
Memo : Bayer CropScience LLC

Printing date : 14.11.2003
Revision date :
Date of last update : 14.11.2003

Number of pages : 27

Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
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. General Information

Id 2231-57-4
Date 14.11.2003

1.0.1 APPLICANT AND COMPANY INFORMATION

Type : manufacturer
Name : Bayer Corporation
Contact person :
Date :
Street : 100 Bayer Road, Building #5
Town : PA 15205-9741 Pittsburgh
Country : United States
Phone :
Telefax :
Telex :
Cedex :
Email :
Homepage :

14.11.2003

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name : 1,3-diamino-2-thiourea
Smiles Code : N(N)C(=S)NN
Molecular formula : C1 H6 N4 S1
Molecular weight : 106.15
Petrol class :

14.11.2003

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type : typical for marketed substance
Substance type : organic
Physical status : solid
Purity : 90.4 % w/w
Colour : white
Odour : slight H₂S

14.11.2003

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1,3-diamino-2-thiourea

14.11.2003

carbonothioic dihydrazide

14.11.2003

TCH

11.11.2003

thiocarbohydrazide

11.11.2003

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1. General Information

Id 2231-57-4
Date 14.11.2003

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2. Physico-Chemical Data

Id 2231-57-4
Date 14.11.2003

2.1 MELTING POINT

Decomposition : yes, at 170 °C
Sublimation :
Method : other: Handbook data
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Reliability : (2) valid with restrictions
Data from Handbook or collection of data

Flag : Critical study for SIDS endpoint
14.11.2003 (1)

2.2 BOILING POINT

Decomposition : yes
Method : other: Handbook data
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Reliability : (2) valid with restrictions
Data from Handbook or collection of data

Flag : Critical study for SIDS endpoint
14.11.2003 (1)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : .002706 hPa at 25 °C
Decomposition :
Method : other (calculated): MPBPWIN v1.41
Year :
GLP : no
Test substance : other TS: molecular structure of Carbonothioic dihydrazide,
CAS # 2231-57-4

Result : Vapor Pressure Estimations (25 deg C):
(Using BP: 232.83 deg C (estimated))
(Using MP: 170.00 deg C (exp database))
VP: 0.00226 mm Hg (Antoine Method)
VP: 0.00203 mm Hg (Modified Grain Method)
VP: 0.00402 mm Hg (Mackay Method)
Selected VP: 0.00203 mm Hg (Modified Grain Method)

Reliability : (2) valid with restrictions
Accepted calculation method

Flag : Critical study for SIDS endpoint
14.11.2003 (2)

2. Physico-Chemical Data

Id 2231-57-4

Date 14.11.2003

2.5 PARTITION COEFFICIENT

Partition coefficient :
Log pow : -2.04 at 25 °C
Method : other (calculated): Log Kow (version 1.67)
Year :
GLP : no
Test substance : other TS: molecular structure of Carbonothioic dihydrazide,
CAS # 2231-57-4

Result : Log Kow (version 1.67 estimate): -2.04

SMILES : N(N)C(=S)NN

CHEM : Carbonothioic dihydrazide

MOL FOR: C1 H6 N4 S1

MOL WT : 106.15

TYPE	NUM	LOGKOW	FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2		-NH2 [aliphatic attach]	-1.4148	-2.8296
Frag	2		-NH- [aliphatic attach]	-1.4962	-2.9924
Frag	1		-NC(=S)N- [thiourea]	1.2905	1.2905
Factor	2		-NH-NH- structure correction	1.1330	2.2660
Const			Equation Constant		0.2290

Log Kow = -2.0365

Reliability : (2) valid with restrictions
Accepted calculation method
Flag : Critical study for SIDS endpoint
14.11.2003

(2)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Description : of very high solubility
Stable :
Deg. product :
Method : other: Handbook data
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Reliability : (2) valid with restrictions
Data from Handbook or collection of data
Flag : Critical study for SIDS endpoint
14.11.2003

(1)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2. Physico-Chemical Data

Id 2231-57-4
Date 14.11.2003

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3. Environmental Fate and Pathways

Id 2231-57-4
Date 14.11.2003

3.1.1 PHOTODEGRADATION

Type : air
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm³
Rate constant : .000000000126 cm³/(molecule*sec)
Degradation : 50 % after 1 hour(s)
Deg. product :
Method : other (calculated): AOP Program (v1.91)
Year :
GLP : no
Test substance : other TS: molecular structure of Carbonothioic dihydrazide,
CAS # 2231-57-4

Reliability : (2) valid with restrictions
Accepted calculation method

Flag : Critical study for SIDS endpoint
14.11.2003 (2)

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media : other: air - water - soil - sediment
Method : other: Level III Fugacity Model
Year :
Remark : Modeling was performed using equal releases (300 kg/hr) and equal
distribution to all compartments.
Result : Level III Fugacity Model (Full-Output):
=====
Chem Name : Carbonothioic dihydrazide
Molecular Wt: 106.15
Henry's LC : 2.76e-012 atm-m3/mole (Henrywin program)
Vapor Press : 0.00203 mm Hg (Mpbpwin program)
Liquid VP : 0.00464 mm Hg (super-cooled)
Melting Pt : 61.3 deg C (Mpbpwin program)
Log Kow : -2.04 (Kowwin program)
Soil Koc : 0.00374 (calc by model)

3. Environmental Fate and Pathways

Id 2231-57-4
Date 14.11.2003

	Mass Amount (%)	Half-Life (hr)	Emissions (kg/hr)
Air	8.95e-005	2.04	300
Water	45.3	360	300
Soil	54.6	360	300
Sediment	0.0755	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (%)	Advection (%)
Air	7.8e-016	0.115	0.00339	0.0128	0.000376
Water	2.23e-017	330	172	36.7	19.1
Soil	9.95e-016	398	0	44.2	0
Sediment	1.86e-017	0.138	0.00572	0.0153	0.000635

Persistence Time: 421 hr
Reaction Time: 520 hr
Advection Time: 2.21e+003 hr
Percent Reacted: 80.9
Percent Advected: 19.1

Reliability : (2) valid with restrictions
Accepted calculation method
Flag : Critical study for SIDS endpoint
14.11.2003

(2)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Result : readily biodegradable
Deg. product :
Method : other: BIOWIN (v4.01)
Year :
GLP : no
Test substance : other TS: molecular structure of Carbonothioic dihydrazide,
CAS # 2231-57-4

Result : BIOWIN (v4.01) Program Results:
=====
SMILES : N(N)C(=S)NN
CHEM : Carbonothioic dihydrazide
MOL FOR: C1 H6 N4 S1
MOL WT : 106.15
----- BIOWIN v4.01 Results -----
Linear Model Prediction : Biodegrades Fast
Non-Linear Model Prediction: Biodegrades Fast
Ultimate Biodegradation Timeframe: Weeks
Primary Biodegradation Timeframe: Days-Weeks
MITI Linear Model Prediction : Does Not Biodegrade Fast
MITI Non-Linear Model Prediction: Does Not Biodegrade Fast

Reliability : (2) valid with restrictions
Accepted calculation method
Flag : Critical study for SIDS endpoint
14.11.2003

(2)

3. Environmental Fate and Pathways

Id 2231-57-4
Date 14.11.2003

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

Species :
Exposure period : at 25 °C
Concentration :
BCF : 3.16
Elimination :
Method : other: BCF Program (v2.15)
Year :
GLP : no
Test substance : other TS: molecular structure of Carbonothioic dihydrazide, CAS # 2231-57-4

Flag : Accepted calculation method
14.11.2003 : Critical study for SIDS endpoint

(2)

3.8 ADDITIONAL REMARKS

4. Ecotoxicity

Id 2231-57-4

Date 14.11.2003

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : other
Species :
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : 24.5
Method : other: ECOSAR v0.99g
Year :
GLP : no
Test substance : other TS: molecular structure of Carbonothioic dihydrazide, CAS # 2231-57-4

Result : ECOSAR v0.99g Class(es) Found

Hydrazines

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Hydrazines	: Fish	96-hr	LC50	24.515
Hydrazines	: Daphnid	48-hr	LC50	17.949
Hydrazines	: Green Algae	144-hr	EC50	1.141
Hydrazines	: Fish		ChV	2.451
Hydrazines	: Daphnid		ChV	1.795
Hydrazines	: Green Algae		ChV	0.285

Reliability : (2) valid with restrictions
Accepted calculation method

14.11.2003

(2)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : other
Species : Daphnia sp. (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
EC50 : 17.9
Method : other: ECOSAR v0.99g
Year :
GLP : no
Test substance : other TS: molecular structure of Carbonothioic dihydrazide, CAS # 2231-57-4

Result : ECOSAR v0.99g Class(es) Found

Hydrazines

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Hydrazines	: Fish	96-hr	LC50	24.515
Hydrazines	: Daphnid	48-hr	LC50	17.949
Hydrazines	: Green Algae	144-hr	EC50	1.141
Hydrazines	: Fish		ChV	2.451
Hydrazines	: Daphnid		ChV	1.795
Hydrazines	: Green Algae		ChV	0.285

Reliability : (2) valid with restrictions
Accepted calculation method

14.11.2003

(2)

4. Ecotoxicity

Id 2231-57-4
Date 14.11.2003

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : other algae
Endpoint :
Exposure period : 144 hour(s)
Unit : mg/l
EC50 : 1.141
Method : other: ECOSAR v0.99g
Year :
GLP : no
Test substance : other TS: molecular structure of Carbonothioic dihydrazide, CAS # 2231-57-4

Result : ECOSAR v0.99g Class(es) Found

Hydrazines

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
=====	=====	=====	=====	=====
Hydrazines	: Fish	96-hr	LC50	24.515
Hydrazines	: Daphnid	48-hr	LC50	17.949
Hydrazines	: Green Algae	144-hr	EC50	1.141
Hydrazines	: Fish		ChV	2.451
Hydrazines	: Daphnid		ChV	1.795
Hydrazines	: Green Algae		ChV	0.285

Reliability : (2) valid with restrictions
Accepted calculation method

14.11.2003

(2)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type : LD50
Value : 41.2 mg/kg bw
Species : rat
Strain : Wistar
Sex : male
Number of animals : 15
Vehicle : other: polyethylene glycol 400
Doses : 2.5, 5, 10, 25, 35, 50, 65, 100 mg/kg
Method : other: similar to Directive 84/449/EEC, B.1
Year :
GLP : no
Test substance : other TS: thiocarbohyrazine, purity = 99.8%

Method : The substance was emulsified in polyethylene glycol 400 and administered to rats using an oral intubation needle. The animals were observed for mortality and morbidity for 14 days. The median lethal dose was calculated using the probit analysis (Fink, et al., "Methods of Information in Medicine" V. 1966).

Remark : Toxic symptoms were fasciculation (muscle spasms) and a deterioration of overall physical condition. Deaths occurred from 1 to 24 hours.

Result : Dose (mg/kg) toxic results death after
 2.5 0/0/15 -
 5.0 0/15/15 -
 10.0 0/15/15 -
 25.0 1/15/15 24 hr
 35.0 6/15/15 2-4 hr
 50.0 10/15/15 2-4 hr
 65.0 13/15/15 2.5 - 3 hr
 100.0 15/15/15 1 - 2 hr

Toxic results = (# deaths / # with symptoms / # animals tested)

NOEL = 2.5 mg/kg

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
 14.11.2003

(3)

Type : LD50
Value : 26.5 mg/kg bw
Species : rat
Strain : Wistar
Sex : female
Number of animals : 15
Vehicle : other: polyethylene glycol 400
Doses : 2.5, 5, 10, 17.5, 25, 35, 50, 100 mg/kg
Method : other: similar to Directive 84/449/EEC, B.1
Year :
GLP : no
Test substance : other TS: thiocarbohyrazine, purity = 99.8%

Method : The substance was emulsified in polyethylene glycol 400 and administered to rats using an oral intubation needle. The animals were observed for mortality and morbidity for 14 days. The median lethal dose was calculated using the probit analysis (Fink, et al., "Methods of Information in Medicine" V. 1966).

5. Toxicity

Id 2231-57-4

Date 14.11.2003

Remark	:	Toxic symptoms were fasciculation (muscle spasms) and a deterioration of overall physical condition. Deaths occurred from 1 to 24 hours.		
Result	:	<u>Dose (mg/kg)</u>	<u>toxic results</u>	<u>death after</u>
		2.5	0/0/15	-
		5.0	0/15/15	-
		10.0	0/15/15	-
		17.5	1/15/15	3.5 hr
		25.0	7/15/15	2-4.5 hr
		35.0	13/15/15	2-4 hr
		50.0	14/15/15	2 hr
		100.0	15/15/15	55min - 1 hr
		Toxic results = (# deaths / # with symptoms / # animals tested)		
		NOEL = 2.5 mg/kg		
Reliability	:	(1) valid without restriction		
Flag	:	Critical study for SIDS endpoint		
14.11.2003				(3)
Type	:	LD50		
Value	:	34.8 mg/kg bw		
Species	:	rat		
Strain	:	Wistar		
Sex	:	male		
Number of animals	:	15		
Vehicle	:	other: polyethylene glycol 400		
Doses	:	2.5, 5, 10, 25, 35, 50, 100 mg/kg		
Method	:	other: similar to Directive 84/449/EEC, B.1		
Year	:			
GLP	:	no		
Test substance	:	other TS: technical grade thiocarbonylazine, purity = 90.4%		
Method	:	The substance was emulsified in polyethylene glycol 400 and administered to rats using an oral intubation needle. The animals were observed for mortality and morbidity for 14 days. The median lethal dose was calculated using the probit analysis (Fink, et al., "Methods of Information in Medicine" V. 1966).		
Remark	:	Toxic symptoms were fasciculation (muscle spasms) and a deterioration of overall physical condition. Deaths occurred from 1 to 24 hours.		
Result	:	<u>Dose (mg/kg)</u>	<u>toxic results</u>	<u>death after</u>
		2.5	0/0/15	-
		5.0	0/15/15	-
		10.0	0/15/15	-
		25.0	1/15/15	1.75 hr
		35.0	8/15/15	1.5 - 3 hr
		50.0	14/15/15	1.5 - 3 hr
		100.0	15/15/15	1 - 2 hr
		Toxic results = (# deaths / # with symptoms / # animals tested)		
		NOEL = 2.5 mg/kg		
Reliability	:	(1) valid without restriction		
14.11.2003				(3)
Type	:	LD50		
Value	:	35.7 mg/kg bw		
Species	:	rat		
Strain	:	Wistar		
Sex	:	female		
Number of animals	:	15		
Vehicle	:	other: polyethylene glycol 400		
Doses	:	2.5, 5, 10, 15, 25, 30, 35, 50, 100 mg/kg		
Method	:	other: similar to Directive 84/449/EEC, B.1		
Year	:			
GLP	:	no		

5. Toxicity

Id 2231-57-4

Date 14.11.2003

Test substance : other TS: technical grade thiocarbohyrazine, purity = 90.4%

Method : The substance was emulsified in polyethylene glycol 400 and administered to rats using an oral intubation needle. The animals were observed for mortality and morbidity for 14 days. The median lethal dose was calculated using the probit analysis (Fink, et al., "Methods of Information in Medicine" V. 1966).

Remark : Toxic symptoms were fasciculation (muscle spasms) and a deterioration of overall physical condition. Deaths occurred from 1 to 24 hours.

Result :

Dose (mg/kg)	toxic results	death after
5.0	0/ 0/15	-
10.0	0/15/15	-
15.0	0/15/15	-
25.0	1/15/15	24 hr
30.0	2/15/15	3.5 hr
35.0	8/15/15	1.5 hr
50.0	14/15/15	1.5 - 2 hr
100.0	15/15/15	1 - 2 hr

Toxic results = (# deaths / # with symptoms / # animals tested)
NOEL = 5 mg/kg

Reliability : (1) valid without restriction
14.11.2003 (3)

5.1.2 ACUTE INHALATION TOXICITY

Type : LC50
Value : 50 mg/m³
Species : rat
Strain : Wistar
Sex : male/female
Number of animals : 10
Vehicle :
Doses : 10, 45, 50, and 60 mg/m³
Exposure time : 4 hour(s)
Method :
Year :
GLP : no
Test substance : other TS: thiocarbohyrazine, purity = 99.8%

Method : Pure TCH was blown by a dust generator into a 20 liter inhalation chamber. The content of TCH in the air of the chamber was determined by weight analysis (membranous filter method). The apparatus was constructed so that exposure to the dust was by inhalation only, no dust touched their bodies. Groups of 10 male and 10 female rats were placed in the chamber for one hour or four hours for a single exposure. The animals were observed for 7 days post-exposure for mortality and morbidity.

Remark : From one to 24 hours after exposure the rats began to develop symptoms in the form of muscle fasciculation (spasms) and general deterioration in physical condition. The spasms were observed during the first 24 hours after exposure and physical condition remained depressed for up to four days. Deaths occurred from one to four days post exposure.

Result :

Conc. (mg/m ³)	toxic results	
	male	female
10	0/ 0/10	0/ 0/10
45	1/10/10	0/10/10
50	4/10/10	4/10/10
60	7/10/10	3/10/10

Toxic results = (# deaths / # with symptoms / # animals tested)
NOEC (4 hrs) = 10 mg/m³

5. Toxicity

Id 2231-57-4

Date 14.11.2003

Reliability	: (2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment													
Flag 14.11.2003	: Critical study for SIDS endpoint	(3)												
Type	: LC50													
Value	: > 75.5 mg/m ³													
Species	: rat													
Strain	: Wistar													
Sex	: male/female													
Number of animals	: 10													
Vehicle	:													
Doses	: 45, 75.5 mg/m ³													
Exposure time	: 1 hour(s)													
Method	:													
Year	:													
GLP	: no													
Test substance	: other TS: thiocarbohyrazine, purity = 99.8%													
Method	: Pure TCH was blown by a dust generator into a 20 liter inhalation chamber. The content of TCH in the air of the chamber was determined by weight analysis (membranous filter method). The apparatus was constructed so that exposure to the dust was by inhalation only, no dust touched their bodies. Groups of 10 male and 10 female rats were placed in the chamber for one hour or four hours for a single exposure. The animals were observed for 7 days post-exposure for mortality and morbidity.													
Remark	: From one to 24 hours after exposure the rats began to develop symptoms in the form of muscle fasciculation (spasms) and general deterioration in physical condition. The spasms were observed during the first 24 hours after exposure and physical condition remained depressed for up to four days. Deaths occurred from one to four days post exposure.													
Result	: <table><thead><tr><th>Conc.</th><th colspan="2">toxic results</th></tr><tr><th>(mg/m³)</th><th>male</th><th>female</th></tr></thead><tbody><tr><td>45</td><td>0/ 0/10</td><td>0/ 0/10</td></tr><tr><td>75.5</td><td>2/10/10</td><td>1/10/10</td></tr></tbody></table> Toxic results = (# deaths / # with symptoms / # animals tested) NOEC (1 hr) = 45 mg/m ³	Conc.	toxic results		(mg/m ³)	male	female	45	0/ 0/10	0/ 0/10	75.5	2/10/10	1/10/10	
Conc.	toxic results													
(mg/m ³)	male	female												
45	0/ 0/10	0/ 0/10												
75.5	2/10/10	1/10/10												
Reliability 14.11.2003	: (2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment	(3)												

5.1.3 ACUTE DERMAL TOXICITY

Type	: LD50	
Value	: > 500 mg/kg bw	
Species	: rat	
Strain	: Wistar	
Sex	: male/female	
Number of animals	:	
Vehicle	: other: polyethylene glycol 400	
Doses	: 500 mg/kg	
Method	:	
Year	:	
GLP	: no	
Test substance	: other TS: thiocarbohyrazine, purity = 99.8%	
Method	: 500 mg pure TCH or technical grade TCH per kg body weight, as a 25%	

5. Toxicity

Id 2231-57-4

Date 14.11.2003

Remark	: emulsion in polyethylene glycol 400, were applied to the skin on the back of each rat. The skin was shaved the previous day. Immediately after application, the site was covered with aluminum foil and wrapped with adhesive elastic bandages. After 24 hours, bandages and foil were removed and the back skin of the animals was cleansed with soap and water (Noakes and Sanderson. Brit. J. Ind. Med. XXVI 1963. p 59). The animals were observed for 7 days.
Reliability	: 24 hours after application, the rats showed a deterioration of general physical condition which lasted 3 to 4 days. No deaths resulted at this dose.
Flag 14.11.2003	: (2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment Critical study for SIDS endpoint (3)
Type	: LD50
Value	: > 500 - mg/kg bw
Species	: rat
Strain	: Wistar
Sex	: male/female
Number of animals	:
Vehicle	: other: polyethylene glycol 400
Doses	: 500 mg/kg bw
Method	:
Year	:
GLP	: no
Test substance	: other TS: technical grade thiocarbohyrazine, purity = 90.4%
Method	: 500 mg pure TCH or technical grade TCH per kg body weight, as a 25% emulsion in polyethylene glycol 400, were applied to the skin on the back of each rat. The skin was shaved the previous day. Immediately after application, the site was covered with aluminum foil and wrapped with adhesive elastic bandages. After 24 hours, bandages and foil were removed and the back skin of the animals was cleansed with soap and water (Noakes and Sanderson. Brit. J. Ind. Med. XXVI 1963. p 59). The animals were observed for 7 days.
Remark	: 24 hours after application, the rats showed a deterioration of general physical condition which lasted 3 to 4 days. No deaths resulted at this dose.
Reliability	: (2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag 14.11.2003	: Critical study for SIDS endpoint (3)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species	: rabbit
Concentration	: 500 mg
Exposure	: Occlusive
Exposure time	: 24 hour(s)
Number of animals	: 1
Vehicle	:
PDII	:
Result	: not irritating

5. Toxicity

Id 2231-57-4

Date 14.11.2003

Classification : not irritating
Method :
Year :
GLP : no
Test substance : other TS: thiocarbohyrazine, purity = 99.8%

Method : 500 mg TCH was applied to 2x2 cellulose pads and placed on the hairless inside of the outer ear of the rabbit. The pads were held in place with bandages for 24 hours. The animals were observed for 7 days post treatment.

Result : No alteration of the treated skin was observed.
14.11.2003 (3)

Species : rabbit
Concentration : 500 mg
Exposure : Occlusive
Exposure time : 24 hour(s)
Number of animals : 1

Vehicle :
PDII :
Result : not irritating
Classification : not irritating

Method :
Year :
GLP : no
Test substance : other TS: technical grade thiocarbohyrazine, purity = 90.4%

Method : 500 mg TCH was applied to 2x2 cellulose pads and placed on the hairless inside of the outer ear of the rabbit. The pads were held in place with bandages for 24 hours. The animals were observed for 7 days post treatment.

Result : No alteration of the treated skin was observed.
14.11.2003 (3)

5.2.2 EYE IRRITATION

Species : rabbit
Concentration : 50 mg
Dose :
Exposure time :
Comment : not rinsed
Number of animals : 1
Vehicle :
Result : not irritating
Classification : not irritating
Method :
Year :
GLP : no
Test substance : other TS: thiocarbohyrazine, purity = 99.8%

Method : 50 mg TCH was applied to the connective tissue sack in the right eye of one rabbit. The rabbits were observed for irritation.

Result : No irritation of the eyelid, connective tissue nor alterations of the cornea were observed.
14.11.2003 (3)

Species : rabbit
Concentration : 50 mg
Dose :
Exposure time :

5. Toxicity

Id 2231-57-4

Date 14.11.2003

Comment : not rinsed
Number of animals : 1
Vehicle :
Result : not irritating
Classification : not irritating
Method :
Year :
GLP : no
Test substance : other TS: technical grade thiocarbohyrazine, purity = 90.4%

Method : 50 mg TCH was applied to the connective tissue sack in the right eye of one rabbit. The rabbits were observed for irritation.

Result : No irritation of the eyelid, connective tissue nor alterations of the cornea were observed.

14.11.2003 (3)

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type : DNA damage and repair assay
System of testing : rat primary hepatocytes
Test concentration : 2.2 µg/ml to 666.7 µg/ml
Cycotoxic concentr. :
Metabolic activation :
Result : positive
Method : EPA OTS 798.5550
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Method : Primary rat liver cell cultures derived from the livers of normal adult male Sprague-Dawley rats were used in this study.
Based on the results of the initial cytotoxicity test, the test article was tested at 6 decreasing dose levels. Three replicate plates seeded with 5.0×10^3 HPC/plate were treated with 666.7 µg/ml to 2.2 µg/ml of test article. DMBA, at 25 µg/ml and 10 µg/ml, was used as the positive control. DMSO, which was used to dissolve the test article and the positive compound, was used as the solvent control.

Result : If the mean net nuclear count is increased by at least five counts over the control, the results for a particular dose level will be considered significant. A test article will be judged positive if it induces a dose-related response and at least one dose produces a significant increase in the average net nuclear grains when compared to that of the control.
The results of the UDS assay indicate that under the test conditions, the test article did cause a significant increase in the mean number of net nuclear grain counts (i.e., an increase of at least 5 counts over the control), at the highest dose level. In addition, a dose response was seen. Therefore, the test article is considered positive in this study.

Reliability : (1) valid without restriction
GLP guideline study

Flag : Critical study for SIDS endpoint

14.11.2003 (4)

5. Toxicity

Id 2231-57-4

Date 14.11.2003

Type : Ames test
System of testing : Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538
Test concentration : 6.7, 10, 33, 67, 100, 333, 667, 1000, 3333, 5000 µg/plate
Cycotoxic concentr. :
Metabolic activation : with and without
Result : positive
Method : EPA OPPTS 870.5265
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Method : Tester strains in use at Microbiological Associates, Inc. received directly from Dr. Bruce Ames, Department of Biochemistry, University of California, Berkeley.

S-9 Homogenate, Liver microsomal enzymes were prepared from male Sprague-Dawley rats that had been injected with Aroclor 1254 at 500 mg/kg.

Due to limited solubility of the test article, the maximum dose tested in the preliminary toxicity determination was 5.0 mg per plate.

Positive Controls; All combinations of positive controls and tester strains plated along with the assay are listed below:

Strain / Activation / Positive Controls / Conc. per Plate

TA98 / + / 2-Aminoanthracene / 4.0 µg

TA98 / - / 2-Nitrofluorene / 5.0 µg

TA100 / + / 2-Aminoanthracene / 4.0 µg

TA100 / - / Sodium Azide / 5.0 µg

TA1535 / + / 2-Aminoanthracene / 4.0 µg

TA1535 / - / Sodium Azide / 5.0 µg

TA1537 / + / 2-Aminoanthracene / 4.0 µg

TA1537 / - / 9-Aminoacridine / 75 µg

TA1538 / + / 2-Aminoanthracene / 4.0 µg

TA1538 / - / 2-Nitrofluorene / 5.0 µg

Result : The test article did cause a weak, reproducible positive increase in TA1535 revertants per plate in two separate experiments (2.5 and 3.1-fold, respectively) in the presence of rat liver microsomes.

In the absence of rat liver microsomes, TA1535 did not demonstrate a positive response.

The remaining tester strains used in this study, TA98, TA100, TA1537 and TA1538, did not demonstrate a positive response either in the presence or absence of rat liver microsomes.

Reliability : (1) valid without restriction
GLP guideline study

Flag : Critical study for SIDS endpoint

14.11.2003

(5)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

9. References

Id 2231-57-4

Date 14.11.2003

- (1) Lide D.R. (ed) 1999- 2000. CRC Handbook of Chemistry and Physics, 80th ed. CRC Press. New York, NY. USA. p 3-111 No. 4033.
- (2) EPIWin Modeling Program. (version 3.11) 2000. Developed by the EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC). copyright 2000 U.S. Environmental Protection Agency
- (3) Groening P. and Kimmerle G. 1975. Thiocarbonylhydrazide: studies on acute toxicity. Bayer AG. Institute of Toxicology. Report No. 5569
- (4) Microbiological Associates, Inc. 1984. Bethesda, Maryland. Tox report # 609.
- (5) Mobay Chemical Corporation. 1985. Stilwell, Kansas. Toxicology Report #619

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT