

201-15095B1

# I U C L I D

## Data Set

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**Existing Chemical** : ID: 126-11-4  
**CAS No.** : 126-11-4  
**CAS Name** : 2-(hydroxymethyl)-2-nitro-1,3-propanediol  
**EINECS No.** : 204-769-5  
**Molecular Formula** : C4H9NO5

**Producer Related Part**  
**Company** : The Dow Chemical Company  
**Creation date** : 11.06.2001

**Substance Related Part**  
**Company** : The Dow Chemical Company  
**Creation date** : 11.06.2001

**Memo** :

**Printing date** : 10.12.2003  
**Revision date** :  
**Date of last Update** : 08.12.2003

**Number of Pages** : 35

**Chapter (profile)** :  
**Reliability (profile)** :  
**Flags (profile)** : ???

# 1. General Information

Id 126-11-4  
Date 10.12.2003

## 1.0.1 OECD AND COMPANY INFORMATION

Type : cooperating company  
Name : ANGUS Chemical Company  
Partner :  
Date :  
Street : 1500 East Lake Cook Road  
Town : 60089 Buffalo Grove, IL  
Country : United States  
Phone : 847-808-3554  
Telefax : 847-808-3710  
Telex :  
Cedex :  
Remark : A wholly owned subsidiary of The Dow Chemical Company.  
28.03.2002

## 1.0.2 LOCATION OF PRODUCTION SITE

Name of Plant : ANGUS Chemical Company  
Street : Louisiana Highway 2  
Town : 71280 Sterlington, LA  
Country : United States  
Phone :  
Telefax :  
Telex :  
Cedex :  
Remark : A subsidiary of The Dow Chemical Company  
13.08.2001

## 1.0.3 IDENTITY OF RECIPIENTS

## 1.1 GENERAL SUBSTANCE INFORMATION

Substance type : organic  
Physical status : solid  
Purity : > 99 % w/w  
20.06.2002

### 1.1.0 DETAILS ON TEMPLATE

Comment : This is the most commercially important member of the category, "nitro alcohols".  
Remark : Molecular Formula: C<sub>4</sub>H<sub>9</sub>NO<sub>5</sub>  
Structural Formula: HOCH<sub>2</sub>C(CH<sub>2</sub>OH)(NO<sub>2</sub>)CH<sub>2</sub>OH  
13.08.2001

### 1.1.1 SPECTRA

## 1.2 SYNONYMS

Tris(hydroxymethyl)nitromethane  
20.06.2002

## 1.3 IMPURITIES

CAS-No : 7732-18-5  
EINECS-No :  
EINECS-Name : water  
Contents : < .2 % w/w  
26.11.2002

## 1.4 ADDITIVES

## 1.5 QUANTITY

### 1.6.1 LABELLING

Labelling : as in Directive 67/548/EEC  
Symbols : Xn  
Nota :  
Specific limits : no  
R-Phrases : (20/22) Harmful by inhalation and if swallowed  
(43) May cause sensitization by skin contact  
S-Phrases : (24) Avoid contact with skin  
(37) Wear suitable gloves

28.03.2002

### 1.6.2 CLASSIFICATION

Classification : as in Directive 67/548/EEC  
Class of danger : harmful  
R-Phrases : (20/22) Harmful by inhalation and if swallowed  
(43) May cause sensitization by skin contact

28.03.2002

## 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. General Information

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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

**Decomposition** : yes at ca. 175 °C  
**Sublimation** : no  
**Method** :  
**Year** :  
**GLP** : no  
**Test substance** : as prescribed by 1.1 - 1.4  
**Remark** : The decomposition of solid TRIS NITRO takes place with the release of significant heat and evolution of gas which can be hazardous.  
**Reliability** : (2) valid with restrictions  
06.12.2002 (1)

### 2.2 BOILING POINT

**Decomposition** : yes  
**Method** :  
**Year** :  
**GLP** :  
**Test substance** :  
**Remark** : Not applicable. This substance decomposes at "melting point".  
**Reliability** : (1) valid without restriction  
07.05.2002

### 2.3 DENSITY

**Type** : relative density  
**Value** : ca. 2 at °C  
**Method** :  
**Year** :  
**GLP** : no  
**Test substance** : as prescribed by 1.1 - 1.4  
**Remark** : The specific gravity of solid TRIS NITRO as a single crystal is about 2.0; however, current product of "solid" TRIS NITRO is obtained by freeze drying. This form of the product varies widely in density. This substance as manufactured is obtained as a solution in water at 50 +/- 3%.  
06.12.2002 (2)

#### 2.3.1 GRANULOMETRY

**Remark** : The solid substance is obtained by "freeze-drying" the 50% solution; it therefore is available commercially in a form of flake.  
**Reliability** : (1) valid without restriction  
06.12.2002 (1)

### 2.4 VAPOUR PRESSURE

**Remark** : No appreciable vapors are generated by the substance itself, exclusive of the vapors formed by decomposition.  
**Reliability** : (1) valid without restriction  
06.12.2002 (1)

## 2. Physico-Chemical Data

Id 126-11-4  
Date 10.12.2003

### 2.5 PARTITION COEFFICIENT

**Log pow** : = 1.06 at 25° C  
**Method** : other (measured): US 40CFR 796.1570  
**Year** : 1991  
**GLP** : yes  
**Test substance** : other TS: 99.69% pure TRIS NITRO  
**Method** : The sample was analyzed by reverse phase-high pressure liquid chromatography using a C-18 column and an ultraviolet detector. The retention time of any substance on the column is a function of the hydrophobicity of the substance. The retention time of the sample was compared to a curve of the log of the retention time vs. the log of the partition coefficient of substances with known partition coefficients.  
**Reliability** : (1) valid without restriction  
14.11.2003 (3)

### 2.6.1 WATER SOLUBILITY

**Value** : other at ° C  
**Qualitative** : of high solubility  
**Pka** : at 25° C  
**PH** : at and ° C  
**Method** : other  
**Year** :  
**GLP** : no  
**Test substance** : as prescribed by 1.1 - 1.4  
**Remark** : Solubility in water is 220 g/100g of water at 20 degrees C.  
The 50% aqueous solution precipitates when cooled below 50 degrees F.  
11.06.2001 (4)

### 2.6.2 SURFACE TENSION

**Remark** : Not applicable for a solid.  
**Reliability** : (1) valid without restriction  
13.08.2001

### 2.7 FLASH POINT

**Value** : > 94° C  
**Type** : closed cup  
**Method** : other  
**Year** :  
**GLP** : no  
**Test substance** : as prescribed by 1.1 - 1.4  
**Remark** : Not applicable for materials which are solids under normal ambient conditions (see melting point). 50% Aqueous solutions did not flash when tested up to 200 degrees F by Tag Closed Cup procedure.  
11.06.2001

### 2.8 AUTO FLAMMABILITY

**Remark** : No data  
**Reliability** : (1) valid without restriction  
13.08.2001

### 2.9 FLAMMABILITY

**Remark** : Not applicable.  
**Reliability** : (1) valid without restriction  
13.08.2001

### 2.10 EXPLOSIVE PROPERTIES

**Result** : not explosive  
**Method** : other  
**Year** : 2000  
**GLP** : no  
**Test substance** : as prescribed by 1.1 - 1.4  
**Remark** : Solid product was subjected to a battery of three tests in order to assess the possibility of explosion.  
**Result** : In the Koenen test, as prescribed by the Transport of Dangerous Goods 1(b)(i), no change in the tube was observed in three trials with the 1 mm orifice.  
The GAP test for solids and liquids was performed according to the procedure of Test 2 a (iii) of the UN Transport of Dangerous Goods Regulations. In two trials, only a slight warping of the witness plate was observed. 2-(Hydroxymethyl)-2-nitro-1,3-propanediol was judged to be insensitive to detonative shock.  
The TIME/PRESSURE test was conducted according to the procedure of Test 2 a (i) of the UN Transport of Dangerous Goods Regulations. In three trials, the test samples failed to reach 300 psig, the pressure which must be reached for any positive finding.  
**Conclusion** : Based on the results of these three tests 2-(hydroxymethyl)-2-nitro-1,3-propanediol is not regarded as an explosive (Class 1) according to transportation regulations.

26.11.2002

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### 2.11 OXIDIZING PROPERTIES

**Result** : no oxidizing properties  
**Remark** : Based upon the chemical structure of this substance it is not an oxidizing agent.

06.08.2001

### 2.12 ADDITIONAL REMARKS

**Memo** : The decomposition which begins at ca. 150 degrees C becomes exothermic and can lead to a deflagration when under confinement.

04.03.2002

### 3. Environmental Fate and Pathways

Id 126-11-4  
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#### 3.1.1 PHOTODEGRADATION

**Type** : air  
**Light source** :  
**Light spect.** : nm  
**Rel. intensity** : based on Intensity of Sunlight  
**Deg. Product** :  
**Method** : other (calculated): Atmospheric Oxidation Program(AOPWIN)  
**Year** : 2002  
**GLP** : no  
**Test substance** :  
**Method** : The estimated atmospheric half-life based on hydroxyl radical attack was obtained using the AOPWIN version 1.90 computer program assuming 12-hour days.  
**Result** : The estimated atmospheric half life was estimated as 5.6 days.  
27.11.2002

#### 3.1.2 STABILITY IN WATER

**Type** : abiotic  
**t1/2 pH4** : at degree C  
**t1/2 pH7** : = 3.4 day at 25 degree C  
**t1/2 pH9** : = 2.4 day at 25 degree C  
**t1/2 pH5** : > 999 day at 25 degree C  
**Deg. Product** : yes  
**Method** : EPA OTS 796.3500  
**Year** : 1993  
**GLP** : yes  
**Test substance** : other TS: 99.69% pure TRIS NITRO  
**Method** : Solutions of TRIS NITRO of concentration 0.001 M were prepared in buffer solutions that were adjusted to pH 5 (0.01 M phthalate), pH 7 (0.01 M phosphate), or pH 9 (0.0025 M borate). Aliquots of the solutions were transferred into 2 mL glass autosampler vials which were then maintained in a darkened incubator for up to 32 days at 25 degrees centigrade.

Individual samples were analyzed at various times post-preparation as follows:

1. TRIS NITRO was determined by HPLC using an Alltech C-18 column eluted with water:methanol equipped with a UV (254 nm) spectrophotometric detector.

2. The pH 7 and 9 solutions were analyzed for formaldehyde using GC equipped with flame-ionization detection.

To determine the effect of formaldehyde on the hydrolytic degradation of TRIS NITRO, a mixture of TRIS NITRO and formaldehyde was added at 0.00035 M:0.002 M to pH 9 solutions and 0.000648 M:0.000983 M to pH 7 buffer solutions. These were then incubated and analyzed as previously described over a period of up to 10 days.

**Result** : TRIS NITRO did not degrade at pH 5. At pH 7 a half life of 3.42 days was determined and at pH 9 the half life was 2.43 days. However, the presence of formaldehyde in closed vials was shown to stabilize TRIS NITRO. This was expected based on the fact that TRIS NITRO is synthesized by a reversible reaction of three moles of formaldehyde with one mole of nitromethane. Stabilization of the TRIS NITRO often was assured in the past by the addition of an acid to adjust the pH of aqueous TRIS NITRO to <2.  
**Reliability** : (1) valid without restriction

### 3. Environmental Fate and Pathways

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07.09.2001

#### 3.1.3 STABILITY IN SOIL

#### 3.2 MONITORING DATA

##### 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

**Type** : fugacity model level I  
**Media** :  
**Air (level I)** : 0  
**Water (level I)** : 99.998  
**Soil (level I)** : .0019  
**Biota (level II / III)** :  
**Soil (level II / III)** : 16.5  
**Method** : other: calculation  
**Year** : 2002  
**Remark** : Regardless of the media to which the TN is released, most of the TN at steady state is in the water phase.  
**Result** : Using the default emissions of equal amounts to soil, air, water and sediment (1000 kg/hr for each) the Level III model predicts that the distribution of TN will be 16.5% in soil, 77% in water, 6.5 % in sediment, and <0.1% in air.  
**Reliability** : (1) valid without restriction  
13.12.2002

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**Type** : adsorption  
**Media** : water - soil  
**Air (level I)** :  
**Water (level I)** :  
**Soil (level I)** :  
**Biota (level II / III)** :  
**Soil (level II / III)** :  
**Method** : other: OECD 121  
**Year** : 2002  
**Method** : HPLC is used to estimate the Adsorption Coefficient of a test material by comparison of the retention time to those of a group of reference compounds. The reference compounds utilized were: acetanilide, phenol, 3-nitrobenzamide, methyl benzoate, naphthalene, 1,2,3-trichlorobenzene, and phenanthrene.  
**Result** : The estimated log Koc for TRIS NITRO is 0.6.  
**Reliability** : (1) valid without restriction  
07.05.2002

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07.05.2002

#### 3.3.2 DISTRIBUTION

#### 3.4 MODE OF DEGRADATION IN ACTUAL USE

### 3. Environmental Fate and Pathways

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#### 3.5 BIODEGRADATION

Type : aerobic  
Inoculum : activated sludge, domestic  
Concentration : 1960mg/l related to related to  
Contact time :  
Degradation : = 13.4 % after 28 day  
Result : other: not readily biodegradable  
Control substance : Benzoic acid, sodium salt  
Kinetic : %  
Deg. Product : %  
Method : OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"  
Year : 2002  
GLP : yes  
Test substance : other TS: 99.69% pure TRIS NITRO  
14.11.2003

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#### 3.6 BOD5, COD OR BOD5/COD RATIO

#### 3.7 BIOACCUMULATION

#### 3.8 ADDITIONAL REMARKS

## 4.1 ACUTE/PROLONGED TOXICITY TO FISH

<b>Type</b>	:	flow through	
<b>Species</b>	:	Cyprinodon variegatus (Fish, estuary, marine)	
<b>Exposure period</b>	:	96 hour(s)	
<b>Unit</b>	:	mg/l	
<b>Analytical monitoring</b>	:	yes	
<b>NOEC</b>	:	m = 501	
<b>LC50</b>	:	m > 501	
<b>Method</b>	:	other: EPA FIFRA Guideline 72-3 (a)	
<b>Year</b>	:	1993	
<b>GLP</b>	:	yes	
<b>Test substance</b>	:	other TS: 99.69% pure TRIS NITRO	
<b>Method</b>	:	Sheepshead minnows ~14 weeks old were maintained in filtered saltwater with a salinity of ~22% at a temperature of 22+/-2 degrees C. Based upon a static range-finding study, test concentrations of nominal(measured) values were chosen for the study as follows: 77.8(64), 130(123), 216(190), 360(356), and 600(501) mg/L. About 1400 mL of each test solution was placed in test chambers and 20 fish were distributed to each test tank. Survival of the fish were then monitored daily and abnormalities of behavior or appearance were noted. Initial dissolved oxygen concentrations ranged from 7.8 to 8.0 mg/L (99 to 101% of saturation) and remained > 6.7 mg/L (>89 % of saturation) throughout the test. The pH values ranged from 8.0 to 8.1 in all control and test solutions throughout the test.	
<b>Result</b>	:	There were no deaths at any test concentration during the 96 hours of the test.	
<b>Reliability</b> 14.11.2003	:	(1) valid without restriction	(10)
<b>Type</b>	:	static	
<b>Species</b>	:	Pimephales promelas (Fish, fresh water)	
<b>Exposure period</b>	:	96 hour(s)	
<b>Unit</b>	:	mg/l	
<b>Analytical monitoring</b>	:	no	
<b>NOEC</b>	:	m = 180	
<b>LC50</b>	:	c = 280	
<b>Method</b>	:	EPA OTS 797.1400	
<b>Year</b>	:	1989	
<b>GLP</b>	:	yes	
<b>Test substance</b>	:	other TS:99.69% TRIS NITRO	
<b>Method</b>	:	Nominal concentrations of 0, 100, 180, 320, 560, and 1000 mg/L were prepared by dissolving the appropriate amount of test substance into 5 gallons of "soft blended" water. The "soft blended" water was prepared by blending hard well water with demineralized water to yield blended water with a total hardness of 40-48 mg/L as CaCO3. The pH of the test water was 7.9 and its dissolved oxygen content was 8.2 mg/L. The study was conducted in duplicate with ten fish per tank for a total of twenty fish per concentration. Water quality parameters of temperature, dissolved oxygen, and pH were monitored and were within acceptable limits during the test.	
<b>Result</b>	:	All exposed fish died at 560 and 1000 mg/L within 24 hours. No fish died at 100 and 180 mg/L. At 320mg/L ten fish died in the first 24 hours, and by 96 hours 14 had died. Only two fish at 320mg/L appeared normal at the end of the test. The LC50 was calculated to be 280 mg/L and the NOEC was 180 mg/L.	
<b>Reliability</b> 14.11.2003	:	(1) valid without restriction	(11)
<b>Type</b>	:	static	
<b>Species</b>	:	Oncorhynchus mykiss (Fish, fresh water)	

## 4. Ecotoxicity

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<b>Exposure period</b>	: 96 hour(s)	
<b>Unit</b>	: mg/l	
<b>Analytical monitoring</b>	: no	
<b>LC50</b>	: c = 410	
<b>Method</b>	: other	
<b>Year</b>	: 1973	
<b>GLP</b>	: no	
<b>Test substance</b>	: no data	
<b>Reliability</b>	: (2) valid with restrictions	
26.11.2002		(12)
<b>Type</b>	: other: predicted value	
<b>Species</b>	:	
<b>Exposure period</b>	:	
<b>Unit</b>	:	
<b>Analytical monitoring</b>	:	
<b>Method</b>	:	
<b>Year</b>	:	
<b>GLP</b>	:	
<b>Test substance</b>	: as prescribed by 1.1 - 1.4	
<b>Remark</b>	: This program only examines the toxicity of the parent compound and would not examine potential break down products such as formaldehyde.	
<b>Result</b>	: The ECOSAR v0.99g program using the Neutral Organics Class and default parameters of Log Kow = -1.66 and Water Solubility = 3,635,000 mg/L was used to predict fish toxicity. The predicted 96-hour LC50 for fish was 309,000 mg/L.	
<b>Reliability</b>	: (2) valid with restrictions	
14.01.2004	2F	

### 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

<b>Type</b>	: static	
<b>Species</b>	: Daphnia magna (Crustacea)	
<b>Exposure period</b>	: 48 hour(s)	
<b>Unit</b>	: mg/l	
<b>Analytical monitoring</b>	: no	
<b>NOEC</b>	: m = 56	
<b>EC50</b>	: c = 80	
<b>Method</b>	: EPA OPP 72-2	
<b>Year</b>	: 1989	
<b>GLP</b>	: yes	
<b>Test substance</b>	: other TS:99.69% pure TRIS NITRO	
<b>Method</b>	: This static study was conducted in 250 mL glass beakers containing 200 mL of daphnid culture/test water. The hardness of the test water was 170 mg/L as CaCO <sub>3</sub> and its pH was 8.1. The dissolved oxygen levels of the test solutions were 8.2 to 8.7 mg/L at the start of the test and were 8.0 to 8.1 mg/L at 48 hours. All test vessels were covered loosely with petri dishes to minimize evaporation. Solutions of 0, 10, 18, 32, 56, 100, and 180 mg/L were prepared in duplicate by weighing the appropriate amount of test article into test vessels. Ten daphnia (first instar <24 hours old) were placed in each vessel to give a total of 20 test organisms per concentration.	
<b>Result</b>	: Immobility was observed only at 100 and 180 mg/L. The 48-hour EC50 was calculated to be 80 mg/L.	
<b>Reliability</b>	: (1) valid without restriction	
14.11.2003		(13)
<b>Type</b>	: flow through	
<b>Species</b>	: Mysidopsis bahia (Crustacea)	

## 4. Ecotoxicity

Id 126-11-4

Date 10.12.2003

**Exposure period** : 96 hour(s)  
**Unit** : mg/l  
**Analytical monitoring** : yes  
**EC0** : m = 95.5  
**Method** : EPA OPP 72-3  
**Year** : 1991  
**GLP** : yes  
**Test substance** : other TS: 99.69% pure TRIS NITRO  
**Method** : Saltwater mysids were exposed to a geometric series of 5 test concentrations, a solvent control, and a negative (salt water) control. The test water was saltwater with a salinity of 24.0 to 26.0 and pH of 7.8 to 8.1. Its dissolved oxygen concentration was 6.0 to 6.8 at the start of the test and was 5.4 to 6.0 after 96 hours. Nominal test concentrations used in the study were 13.0, 21.6, 36.0, 60.0, and 100 mg of TRIS NITRO per liter based on the results of a range-finding study. Based on the analyses of each dosage level at the beginning and end of the exposure period the mean measured test concentrations were 11.9, 22.6, 35.8, 54.3, and 95.5 mg/L. Ten shrimp were placed in each chamber. Two chambers at each concentration were utilized so that a total of 20 shrimp were exposed at each dose. Observation of mortality, as well as treatment related effects were made at 17, 24, 48, 72, and 96 hours. The LC50 was calculated based on mortalities observed at various intervals of time.

**Result** : No mortality was observed in this study. The 96-hour EC50 is >95.5 mg/L, which is also an EC0 for this study.

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

(14)

**Type** : flow through  
**Species** : other aquatic mollusc: Crassostrea virginica  
**Exposure period** : 96 hour(s)  
**Unit** : mg/l  
**Analytical monitoring** : yes  
**NOEC** : m = 1.3  
**EC50** : m = 27.8  
**Method** : EPA OTS 797.1800  
**Year** : 1991  
**GLP** : yes  
**Test substance** : other TS: 99.69% pure TRIS NITRO  
**Method** : Oysters were exposed to a geometric series of five test concentrations, a negative (unfiltered saltwater) control, and a solvent control for a period of 96 hours. The saltwater had a salinity of 25, a pH of 7.9 to 8.0, and the dissolved oxygen content of the test solutions was 6.1 to 6.6 mg/L over the 96-hour period of the test. Nominal test concentrations selected for the study were 1.3, 3.2, 8.0, 20, and 50 mg of TRIS NITRO/L. The two lowest concentrations were below the limit of detection of the analytical method. However, the mean measured concentrations for the other test solutions were 9.2, 18.6, and 52.4 mg/L which were in close agreement to the nominal concentrations. Immediately prior to test initiation, 2-3 mm of the shell periphery were removed from each oyster using a motorized grinder. Twenty oysters were placed in chambers containing each test concentration. The flow of unfiltered salt water into each chamber was approximately 1 L per oyster per hour. Algal cells were provided to the solutions to maximize growth during the test. Measurement of shell deposition for each oyster was made at 96 hours and used to calculate the EC50 for inhibition of shell deposition.

**Result** : Shell deposition was inhibited at all TRIS NITRO concentrations except 1.3 mg/L. Shell deposition for the negative and solvent controls was ca. 4 mm in 96 hours. Inhibition in deposition varied from 6% at 3.2 mg/L to 71.4 % at 50 mg/L. The 96-hour EC50 was calculated to be 27.8 mg/L.

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

(15)

## 4. Ecotoxicity

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10.08.2001

**Type** : other: predicted value  
**Species** :  
**Exposure period** :  
**Unit** :  
**Analytical monitoring** :  
**Method** :  
**Year** :  
**GLP** :  
**Test substance** : as prescribed by 1.1 - 1.4  
**Remark** : This program only examines the toxicity of the parent compound and would not examine potential break down products such as formaldehyde.  
**Result** : The ECOSAR v0.99g program using the Neutral Organics Class and default parameters of Log Kow = -1.66 and Water Solubility = 3,635,000 mg/L was used to predict daphnia toxicity. The predicted 48-hour LC50 for daphnia was 257,000 mg/L.  
**Reliability** : (2) valid with restrictions 2F  
2F

14.01.2004

### 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

**Species** : Selenastrum capricornutum (Algae)  
**Endpoint** : growth rate  
**Exposure period** : 96 hour(s)  
**Unit** : mg/l  
**Analytical monitoring** : yes  
**NOEC** : c = .269  
**EC50** : c = .656  
**Method** : OECD Guide-line 201 "Algae, Growth Inhibition Test"  
**Year** : 2002  
**GLP** : yes  
**Test substance** : other TS: 99.69% pure TRIS NITRO  
**Method** : Tris Nitro was added to 250 mL erlenmeyer flasks containing approximately 10,000 cells/mL of Selenastrum capricornutum in algal assay medium specifically prepared using deionized water as designated by the EPA guideline. Its final pH was adjusted to pH 7.0 to 7.5. The measured levels of TRIS NITRO in the flasks was 0, 0.017, 0.042, 0.109, 0.269, 0.654, 1.61, and 4.50 mg/L. After 96 hours of exposure at 23.9 C, algal cell densities were determined by electron particle counting using a Coulter Multisizer.  
**Result** : The 3- and 4-day growth rate EC50 values, based on mean analyzed concentrations, were both greater than 4.50 mg/L.  
The 3- and 4-day percent inhibition EC50 values, based on mean analyzed concentrations, were 0.479 mg/L and 0.566 mg/L respectively  
The 3- and 4-day cell density EC25 values, based on mean analyzed concentrations, were 0.127 mg/L and 0.177 mg/L respectively.  
The 3- and 4-day cell density EC50 values, based on mean analyzed concentrations, were 0.468 mg/L and 0.651 mg/L respectively.  
The statistically derived 3- and 4-day no-observed-effect concentrations (alpha=0.05), based on mean analyzed concentrations, were both 0.269 mg/L.  
**Reliability** : (1) valid without restriction  
14.11.2003

(16)

**Species** :  
**Endpoint** : other: predicted value  
**Exposure period** :  
**Unit** :  
**Analytical monitoring** :

**Method** :  
**Year** :  
**GLP** :  
**Test substance** : as prescribed by 1.1 - 1.4  
**Remark** : This program only examines the toxicity of the parent compound and would not examine potential break down products such as formaldehyde.  
**Result** : The ECOSAR v0.99g program using the Neutral Organics Class and default parameters of Log Kow = -1.66 and Water Solubility = 3,635,000 mg/L was used to predict algae toxicity. The predicted 96-hour LC50 for algae was 130,000 mg/L.  
**Reliability** : (2) valid with restrictions  
 2F  
 14.01.2004

#### 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 SOIL DWELLING ORGANISMS

##### 4.6.2 TOXICITY TO TERRESTRIAL PLANTS

##### 4.6.3 TOXICITY TO OTHER NON-MAMM. TERRESTRIAL SPECIES

**Species** : *Anas platyrhynchos* (avian)  
**Endpoint** : mortality  
**Exposure period** : 5 day  
**Unit** : ppm  
**Method** :  
**Year** : 1978  
**GLP** : no  
**Test substance** : other TS: 50% TRIS NITRO in water  
**Method** : Eight ducklings, 15 days old, were placed randomly into each of 9 separate pens. Groups 1, 2, and 3 were control animals. Group 4 received a diet containing 80,000 ppm of TRIS NITRO 50%. The diets of the remaining groups contained the following levels of TRIS NITRO 50%: Group 5--40,000; Group 6--20,000; Group 7--10,000; Group 8--5,000; Group 9--2500 ppm. Following feeding for 5 days ad libitum with the treated feed, all animals were placed on the standard diet for a 3-day post treatment period. Weights were measured at initiation, after 5 days, and at termination (8 days). Feed consumption was monitored throughout the study and each pen was observed daily for signs of toxic effects and mortality.  
**Result** : No mortality attributable to the test substance was observed during the initial 8 day feeding period. Within 24 hours of placement on the treated diets, all ducks at 80,000 and 40,000 ppm had a lack of coordination with difficulty in walking and the heads swinging from side to side. Occasionally, the duck's heads would reflect backward until its skull would be resting on the back and the duck would walk backwards. At 20,000 ppm, these same symptoms appeared 96 hours after start in three ducks only. All ducks were normal at all other dosages.

Because of the above symptoms, the study was extended for twelve additional days. By day 15 only 3 ducks at 80,000 ppm and one at 40,000 ppm were still affected. All ducks at 20,000 ppm appeared normal on day 14. Histopathological examination of the brains of those animals still affected showed focal loss of Purkinje cells of the cerebellum and edema in cerebellum.

<b>Reliability</b> 14.11.2003	:	The 8-day dietary LC50 was greater than 80,000 ppm in the diet. (2) valid with restrictions	(17)
<b>Species</b>	:	Colinus virginianus (avian)	
<b>Endpoint</b>	:	mortality	
<b>Exposure period</b>	:		
<b>Unit</b>	:		
<b>Method</b>	:		
<b>Year</b>	:	1978	
<b>GLP</b>	:	no	
<b>Test substance</b>	:	other TS: 50% TRIS NITRO in water	
<b>Method</b>	:	Bobwhite quail, 10 days old, were placed randomly into 5 separate pens of 10 birds each. Groups 1, and 2 were control animals. Group 3 received a diet containing 5,000 ppm of TRIS NITRO 50%. The diets of the remaining groups contained the following levels of TRIS NITRO 50%: Group 4--2500 ppm; Group 5--1250 ppm. Following a 5 day ad libitum period with the treated feed, all animals were placed on the standard diet for a 3-day post treatment period. Weights were measured at initiation, after 5 days, and at termination (8 days). Feed consumption was monitored throughout the study and each pen was observed daily for signs of toxic effects and mortality.	
<b>Result</b>	:	No mortality occurred during this study. Feed consumption and body weight gain were normal for all groups. No signs of toxicity or symptoms suggestive of toxicity were observed. The dietary LC50 was greater than 5000 ppm in the diet.	
<b>Reliability</b> 14.11.2003	:	(2) valid with restrictions	(18)
13.08.2001			

#### 4.7 BIOLOGICAL EFFECTS MONITORING

#### 4.8 BIOTRANSFORMATION AND KINETICS

#### 4.9 ADDITIONAL REMARKS

## 5.1.1 ACUTE ORAL TOXICITY

<b>Type</b>	: LD50
<b>Species</b>	: rat
<b>Strain</b>	: other: Cox SD
<b>Sex</b>	: male/female
<b>Number of animals</b>	:
<b>Vehicle</b>	: water
<b>Value</b>	: = 990 - 1000 mg/kg bw
<b>Method</b>	: other: IMC Toxicology Laboratory Protocol
<b>Year</b>	: 1979
<b>GLP</b>	: no
<b>Test substance</b>	: other TS: >99 %
<b>Method</b>	: This study was conducted using the IMC Toxicology Laboratory Standard protocol which is similar to EPA guidelines. Ten male and ten female rats were used at each dose level. Doses were at 0, 700, 900, 1300, 1600, and 2200 mg/kg body weight. The animals were weighed on days 1, 7, and 14 of the study. After 14 days the surviving rats were sacrificed and examined for gross pathology.
<b>Result</b>	: One male rat in the 900 mg/kg group and two male rats in the 1300 mg/kg group died. Almost equal numbers of both sexes died in the 1600 mg/kg (5 total) and 2200 mg/kg (14 total) groups. The weight gain for all dosed animals was the same as was that of the controls except for that of the high dose males. At 1300 mg/kg and higher, dosed animals developed tremors within 24 hours and survivors returned to normal within 2 to 6 days. Animals that died had pale livers and spleens.
<b>Test substance</b>	: 53.1% in water
<b>Conclusion</b>	: The LD50 for this substance in solution was 1860 to 1890 mg/kg body weight. Based on the concentration of this aqueous form of the test article the LD50 of the active ingredient is 990 to 1000 mg/kg body weight.
<b>Reliability</b>	: (2) valid with restrictions
08.12.2003	

(19)

## 5.1.2 ACUTE INHALATION TOXICITY

<b>Type</b>	: LC50
<b>Species</b>	: rat
<b>Strain</b>	: Sprague-Dawley
<b>Sex</b>	: male/female
<b>Number of animals</b>	: 10
<b>Vehicle</b>	: other: none
<b>Exposure time</b>	: 4 hour(s)
<b>Value</b>	: > 2.12 mg/l
<b>Method</b>	: EPA OPP 81-3
<b>Year</b>	: 1995
<b>GLP</b>	: yes
<b>Test substance</b>	: other TS: >99.69 % TRIS NITRO
<b>Remark</b>	: Exposure was to a dust of test article ground to a fine particle size. The gravimetric chamber concentration was 2.12 mg/L. The mass median aerodynamic diameter was estimated to be 3.8 microns based on graphic analysis of the particle size distribution as measured with an Anderson Cascade Impactor. After whole-body exposure the rats were observed for 14 days prior to terminal sacrifice and necropsy.
<b>Result</b>	: One male and one female died within four days of exposure. During the first hour of exposure, irregular respiration, hunched posture, and hypoactivity were noted. Within several days of the exposure, facial staining, piloerection, red nasal discharge and reduced feed consumption

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and fecal volume were observed. All surviving rats recovered from the above conditions by day 6 and gained weight over the 14-day observation period. Gross necropsy of the decedents revealed discoloration of the lungs, liver, gastro-intestinal tract, gaseous distention of the stomach and rigor mortis. Gross necropsy findings at terminal sacrifice were unremarkable.

**Reliability** : (1) valid without restriction  
08.12.2003 (20)

**Type** : LC50  
**Species** : rat  
**Strain** : Sprague-Dawley  
**Sex** : male/female  
**Number of animals** : 10  
**Vehicle** : other: none  
**Exposure time** : 4 hour(s)  
**Value** : 2.4 mg/l  
**Method** : EPA OPP 81-3  
**Year** : 1980  
**GLP** : yes  
**Test substance** : other TS: 54.82% TRIS NITRO in water  
**Method** : Groups of Sprague-Dawley rats (5 males and 5 females in each) were exposed for 4 hours to TRIS NITRO concentrate at actual measured concentrations of 4.7, 2.7, 1.9, 1.8, 0.67, and 0 mg/L. The aerosol had an equivalent aerodynamic diameter of 2.4 micro meters with a geometric standard deviation of 2.0. After exposure, the rats were observed for 14 days prior to sacrifice and necropsy.

**Result** : Mortality for the various groups was as follows: 4.7 mg/L - 80%; 2.7 mg/L - 70%; 1.9 mg/L - 50%; 1.8 mg/L - 20%; 0.67 mg/L and controls - 0. Mortality in the various dose groups occurred within the first 6 days post-exposure.

During exposure nasal discharge was observed in almost all rats dosed at 2.7 mg/L or greater. At 1.8 mg/L, half of the animals exhibited nasal discharge; this effect seemed to be compound related. Four animals at 4.7 mg/L, two at 2.7 mg/L, and 3 at 0.67 mg/L exhibited dyspnea.

During the post-exposure period, the following clinical signs were noted in both males and females exposed: dyspnea, red matter on the face, ataxia, and death. The incidence of these findings began with the 1.9 mg/L group and increased with dose.

The only compound related finding in the histopathological examination were in the kidneys. All treatment groups except for low dose group (0.67 mg/L) were found to exhibit tubular nephrosis. Very slight to moderate nephritis, nephrolithiasis, papillitis, and pyelitis were found in all treatment groups. The severity of these effects was slightest for the low dose group.

**Reliability** : (1) valid without restriction  
14.11.2003 (21)

### 5.1.3 ACUTE DERMAL TOXICITY

**Type** : LD0  
**Species** : rat  
**Strain** : Sprague-Dawley  
**Sex** : male/female  
**Number of animals** : 10  
**Vehicle** : water  
**Value** : > 5000 mg/kg bw  
**Method** : EPA OPP 81-2

<b>Year</b>	:	1998	
<b>GLP</b>	:	yes	
<b>Test substance</b>	:	other TS: >99.96% TRIS NITRO	
<b>Method</b>	:	Five thousand milligrams of test substance per kilogram body weight was moistened to a dry paste with distilled water and applied to the skin of 10 healthy rats for 24 hours. The treated areas were covered with a gauze pad during exposure after which residual material was removed with a damp towel. The animals were observed for signs of gross toxicity and behavioral changes at least once a day for 14 days. Bodyweights were recorded prior to exposure and on days 7 and 14. Necropsies were performed on all animals at terminal sacrifice.	
<b>Result</b>	:	All animals survived, gained weight, and appeared active and healthy. There were no signs of gross toxicity, skin irritation, adverse clinical effects. Gross necropsy findings at terminal sacrifice were generally unremarkable.	
<b>Reliability</b> 14.11.2003	:	(1) valid without restriction	(22)
<b>Type</b>	:	LD0	
<b>Species</b>	:	rabbit	
<b>Strain</b>	:	New Zealand white	
<b>Sex</b>	:	male/female	
<b>Number of animals</b>	:	10	
<b>Vehicle</b>	:	physiol. saline	
<b>Value</b>	:	> 2000 mg/kg bw	
<b>Method</b>	:	other: IMC Toxicology Protocol No. 5	
<b>Year</b>	:	1981	
<b>GLP</b>	:	no	
<b>Test substance</b>	:	other TS: >99% TRIS NITRO	
<b>Method</b>	:	Abdomens of ten rabbits (5 of each sex) were shaved and then abraded with a blunt syringe. The prepared area was then spread with enough finely ground test article to provide a dose of 2000 mg/kg bodyweight. The test article was wet with saline to form a paste which was then covered and left on the skin for 24 hours after which the cover and test material were removed. Animals were then held for 14 days before sacrifice and necropsy.	
<b>Result</b>	:	There were no deaths, all rabbits gained weight normally, and exhibited no effects attributable to treatment.	
<b>Reliability</b> 14.11.2003	:	(2) valid with restrictions	(23)
20.07.2001			

#### 5.1.4 ACUTE TOXICITY, OTHER ROUTES

##### 5.2.1 SKIN IRRITATION

<b>Species</b>	:	rabbit
<b>Concentration</b>	:	undiluted
<b>Exposure</b>	:	Semiocclusive
<b>Exposure time</b>	:	4 hour(s)
<b>Number of animals</b>	:	6
<b>PDII</b>	:	0
<b>Result</b>	:	slightly irritating
<b>EC classification</b>	:	not irritating
<b>Method</b>	:	EPA OPP 81-5
<b>Year</b>	:	1998
<b>GLP</b>	:	yes
<b>Test substance</b>	:	other TS: >99.96% TRIS NITRO

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**Method** : Five-tenths of a gram of test substance was moistened to a dry paste with distilled water and applied to the skin of 6 healthy rabbits (3 of each sex) for 4 hours. Following exposure, dermal irritation was evaluated by the method of Draize et al at 1, 24, 48, and 72 hours.

**Result** : Draize scores at all observation times were zero. Thus the material was not irritating to the skin.

**Reliability** : (1) valid without restriction  
14.11.2003 (24)

### 5.2.2 EYE IRRITATION

**Species** : rabbit  
**Concentration** : undiluted  
**Dose** : .1 other: gm  
**Exposure Time** : 24 hour(s)  
**Comment** : other: Six rabbits treated and left alone; six others had eye rinsed after 20-30 seconds.

**Number of animals** : 12  
**Result** : not irritating  
**EC classification** : not irritating  
**Method** : other: IMC Toxicity Laboratory protocol No. 2  
**Year** : 1982  
**GLP** : no  
**Test substance** : other TS: > 95% TRIS NITRO  
**Method** : One-tenth of a gram of finely ground test material was placed in the left eye of 12 rabbits. The eyes of 6 rabbits were left untreated and the eyes of the other 6 were irrigated with lukewarm tap water after 20-30 seconds. At 24 hours and on the 7th day, a drop of sodium fluorescein was placed on the cornea of each treated eye and excess was flushed away with sterile saline. Eyes were examined at 24, 48, 72 hours and at 7 days.

**Result** : No lesions were observed following fluorescein treatment. At 24 hours, the average score for the unwashed eyes was 2.0 (redness of the conjunctivae). At 48 hours the average score had dropped to 0.3. Scores at 72 hours and later were zero. Washed eyes exhibited even lower scores: 1.3 at 24 hours and zero thereafter.

**Reliability** : (2) valid with restrictions  
14.11.2003 (25)

### 5.3 SENSITIZATION

**Type** : Guinea pig maximization test  
**Species** : guinea pig  
**Concentration** : Induction 50 % active substance intracutaneous  
Induction 25 % active substance occlusive epicutaneous  
Challenge 25 % active substance occlusive epicutaneous

**Number of animals** : 24  
**Vehicle** : water  
**Result** : not sensitizing  
**Classification** : not sensitizing  
**Method** : OECD Guide-line 406 "Skin Sensitization"  
**Year** : 1997  
**GLP** : yes  
**Test substance** : other TS: 99.69% pure TRIS NITRO  
**Method** : The application sites of 24 Guinea pigs were prepared by clipping a 5 x 7 cm area of skin on the shoulder area free of hair (on days 0 and 7). On day 23, a 4 x 4 cm area on the flank was so clipped.

Irritancy was determined in 5 animals total. Intradermal treatment caused

	irritation at 50% concentration and topical treatment caused irritation at 70% (but not at 50%).	
	Induction thus was conducted intradermally on day 0 with: <ol style="list-style-type: none"> <li>1. 0.1mL Freund's Complete Adjuvant (FCA) 1:1 w water</li> <li>2. 0.1mL test article</li> <li>3. 0.1mL test article 1:1 w FCa</li> </ol> The test article was 50% TRIS NITRO or 0.1% DNCB (dinitrochlorobenzene) in 95% EtOH as the positive control. Water was the negative control. On day 7 the induction phase continued with a topical application of these same solutions which was left in place for 48 hours.	
	Challenge was conducted on day 23 with either 25% TRIS NITRO, water, or 0.1% DNCB in EtOH under occlusive patch. After 24 hours exposure the patches were removed and the treated area were scored for erythema and edema after 24 , 48 and 72 hours.	
<b>Result</b>	: There were no clinical signs of toxicity during the test and test animals gained weight in a manner comparable to that of the controls. The scores for all ten animals exposed to TRIS NITRO and the five the negative control (water) animals were zero for both erythema and edema at all evaluations times. All the animals exposed to DNCB exhibited irritation at all evaluations.	
<b>Reliability</b> 14.11.2003	: TRIS NITRO was nonsensitizing under conditions of this test. (1) valid without restriction	(26)
<b>Type</b>	: other: Intradermal method of Landsteiner and Jacobs	
<b>Species</b>	: guinea pig	
<b>Number of animals</b>	: 10	
<b>Vehicle</b>	: water	
<b>Result</b>	: not sensitizing	
<b>Classification</b>	: not sensitizing	
<b>Method</b>	: other: see J. Exper. Med., Vol.61:643-656 (1935).	
<b>Year</b>	: 1980	
<b>GLP</b>	: no	
<b>Test substance</b>	: other TS: 56.78% TRIS NITRO in water	
<b>Method</b>	: Thirty male guinea pigs weighing 250-300 g were divided into three groups of 10 each. The animals backs and flanks were shaved free of hair. Group I was intradermally injected with 0.05 mL of 0.5% solution of active TRIS NITRO in distilled water. Group II (positive control) was similarly injected with 0.05 mL of 0.3% DNCB alcoholic solution (4%). Group III (negative control) was injected with 0.05 mL of saline. After 24 hours the injected sites were scored for erythema and edema. At 48 hours, the intradermal injection procedure was repeated for each group with 0.1 mL of each solution 3 times a week for 3 weeks until a total of 10 injections had been made.	
	After the last injection, the animals were allowed to rest for 2 weeks. On the first day of the following week, animals in each group were challenged intradermally with 0.1 mL of their respective solution. In addition, Group III animals also were challenged with the TRIS NITRO and DNCB solutions. At the end of 24 and 48 hours, the injected sites were scored for inflammatory skin reactions according to the system of Draize.	
<b>Result</b>	: During the induction phase or at the challenge, none of the treated (Group I) or the control animals (Group III) showed any skin reactions. The Group II animals showed mild to severe skin reactions during the induction phase and at the challenge.	
<b>Reliability</b> 14.11.2003	: (2) valid with restrictions	(27)

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<b>Type</b>	:	Guinea pig maximization test
<b>Species</b>	:	guinea pig
<b>Concentration</b>	:	Induction 10 % intracutaneous Challenge undiluted occlusive epicutaneous
<b>Number of animals</b>	:	24
<b>Vehicle</b>	:	water
<b>Result</b>	:	sensitizing
<b>Classification</b>	:	sensitizing
<b>Method</b>	:	OECD Guide-line 406 "Skin Sensitization"
<b>Year</b>	:	1998
<b>GLP</b>	:	yes
<b>Test substance</b>	:	other TS: 40% TRIS NITRO in water as manufactured
<b>Method</b>	:	Method followed was the same as described previously except that no concurrent positive control animals were utilized. Intradermal induction was conducted with 0.1 mL of test article diluted 1:9 with water. Topical induction was with undiluted test article and challenge was conducted with undiluted test article and with 75% test article. Topical application was by a 40 mm x 20 mm filter paper saturated with solution.
<b>Remark</b>	:	The positive result in this test was a result of the 0.7% of free formaldehyde present in this product as manufactured in Europe. Unlike the crystalline, pure grade of TRIS NITRO, 40% TRIS NITRO contains more than 0.2% of free formaldehyde. Also, the degree of reaction was not unlike that observed in the topical induction phase of the where undiluted test material caused similar reactions at 24 hours post-exposure.
<b>Result</b>	:	The test material produced an 80% sensitization rate and was classified as a strong sensitizer.
<b>Reliability</b>	:	(2) valid with restrictions
14.11.2003		

(28)

### 5.4 REPEATED DOSE TOXICITY

<b>Species</b>	:	rat
<b>Sex</b>	:	male/female
<b>Strain</b>	:	other: Crl:CD BR
<b>Route of admin.</b>	:	dermal
<b>Exposure period</b>	:	Six hours per day, five days per week for 13 weeks.
<b>Frequency of treatment</b>	:	Daily except weekends
<b>Post obs. period</b>	:	None
<b>Doses</b>	:	To 15 males and 15 females each at doses of 0, 250, 500, and 1000 mg/kg/day
<b>Control group</b>	:	yes, concurrent vehicle
<b>NOAEL</b>	:	> 1000 mg/kg bw
<b>Method</b>	:	EPA OPP 82-3
<b>Year</b>	:	1989
<b>GLP</b>	:	yes
<b>Test substance</b>	:	other TS:99.69% pure TRIS NITRO
<b>Method</b>	:	An area of approximately 20-25% of the surface area of the rats was clipped free of hair 24 hours before the first application to the skin. The test material was applied as a paste wet with water (0.05, 0.1, and 0.2 mL for the 250, 500, and 1000 mg/kg/day groups respectively). The test material was spread over 6% of the body area with the 250 mg/kg group and over 9% of the body area with the 500 and 1000 mg/kg groups. The control group received deionized water spread over 9-10% of the body area. Animals were dosed daily and the exposed areas covered with a gauze binder secured with tape. After six hours the gauze was removed and the exposed areas washed. All rats wore Elizabethan collars to prevent ingestion of the test material.

<b>Remark</b>	: Animals were inspected at least twice daily for mortality and overt signs of toxicity. Individual body weights and food consumption were measured weekly beginning one week before initiation of dosing. Ophthalmological examinations were conducted and hematology and clinical chemistry were checked prior to initiation of dosing and just prior to terminal sacrifice. Urinalysis was conducted on all rats during week 12 of the study. All animals were subject to gross and microscopic pathological examination at termination of the study.
<b>Result</b>	: <b>Reproductive Toxicity:</b> Males - At sacrifice, there was no significant difference in the weight of the testes of the high dose rats in comparison to the weight of the testes of the controls; neither was there significant difference in their relative weight versus body weight. Histopathologic findings for all animals examined (i.e. controls and high dose rats) were that the testes of all animals were "within normal limits".  Females - Again, the weights (absolute and relative) of the ovaries of all animals were not significantly different. The only histopathologic finding was a minimal cyst in the ovary of one high-dose rat. : The only mortality during the course of the study was for one control female which died in week 4. This death was attributed to an injury sustained several weeks prior to death. No clinical signs of toxicity were observed. Although the application sites were discolored yellow throughout the study, microscopic examination of skin samples from the control and high dose group animals did not reveal any adverse effects related to exposure. The test material was essentially nonirritating. No compound related adverse effects were noted on body weights or body weight gain, food consumption, hematology or serum chemistry parameters, urinalysis parameters, absolute or relative organ weights, ophthalmoscopic findings, lesions at gross necropsy, or nonneoplastic histologic lesions.
<b>Reliability</b> 14.11.2003	: (1) valid without restriction

(29)

**5.5 GENETIC TOXICITY 'IN VITRO'**

<b>Type</b>	: Ames test
<b>System of testing</b>	: Tested in Salmonella typhimurium, TA98, TA100, TA1535, TA1537, and TA1538.
<b>Concentration</b>	: 0.1, 0.2, 0.3, 0.5, and 1 mg/plate
<b>Cycotoxic conc.</b>	: 2 mg/plate
<b>Metabolic activation</b>	: with and without
<b>Result</b>	: negative
<b>Method</b>	: EPA OTS 798.5265
<b>Year</b>	: 1988
<b>GLP</b>	: yes
<b>Test substance</b>	: other TS: 99.69% TRIS NITRO
<b>Result</b>	: The test article was found to be toxic at doses greater than 1.0 mg/plate in a preliminary study. None of the dose levels tested induced an increase in revertants in comparison with the vehicle control.
<b>Test condition</b>	: All dose levels with and without activation were run simultaneously in triplicate. The negative control was the vehicle (water). Sodium azide (for TA-1535 & TA-100), 2-nitrofluorene (for TA-1538 & TA-98), 9-aminoacridine (for TA-1537), and 2-amino-anthracene (all strains), the positive controls, all exhibited the expected positive response.
<b>Reliability</b> 14.11.2003	: (1) valid without restriction
<b>Type</b>	: Chromosomal aberration test

(30)

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**System of testing** : Chinese Hamster Ovary  
**Concentration** : 0.125, 0.25, 0.5, 1.0, and 2.0 mg/mL  
**Cycotoxic conc.** : 0.1 mg/mL without S9 and 1 mg/mL with S9  
**Metabolic activation** : with and without  
**Result** : negative  
**Method** : EPA OTS 798.5375  
**Year** : 1991  
**GLP** : yes  
**Test substance** : other TS: 99.69% TRIS NITRO  
**Method** : Following cytotoxicity (dose-selection) testing, duplicate cultures of CHO cells were exposed for 8 hours in the absence of activation, but only 2 hours in the presence of a metabolic activation system consisting of the microsomal fraction prepared from the livers of male Sprague-Dawley rats pretreated with Arochlor 1254, plus NADP(H)-generating co-factors (S9). Following treatment, cell cultures were washed and reincubated in fresh medium for up to 20 hours, the last 1 to 2 hours of which were in the presence of mitotic-arresting (C-metaphase) alkaloid, Colcemid. Cells were then harvested (by mitotic shake-off), onto glass microscope slides, expanded in hypotonic buffer (30 mM KCl, 10 mM sodium citrate), fixed in Carnoy (3 parts methanol: 1 part glacial acetic acid), and stained with 5 to 10 percent Giemsa. Positive controls were run concurrently employing the clastogens, mitomycin C (MMC) and cyclophosphamide (CP), under non-activated and activated conditions, respectively.

At least 50 cells per blind-coded slide were scored for the conventional array of structural chromatid and chromosome aberrations; chromosome numbers also were recorded as a measure of numerical aberrations. Chromosome data were analyzed by Chi-Square, with significance set at  $p < 0.05$ .

**Result** : 2-(Hydroxymethyl)-2-nitro-1,3-propanediol was lethal at 10,000 micrograms per mL without S9 activation and at 1000 micrograms per mL with S9 activation. Lower doses provided relative survival values between 50% and 60 % of the solvent control. Hence 2000 micrograms per mL was chosen as the high dose.

No increases in chromosome aberrations were found for the test material either with or without S9 activation. By contrast, both clastogens induced significantly positive responses.

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

(31)

**Type** : Unscheduled DNA synthesis  
**System of testing** :  
**Concentration** : Tested at 10, 50, 100, and 500 micrograms per mL as well as 1 and 10 mg/mL.  
**Cycotoxic conc.** : In the preliminary test, there was no apparent cytotoxicity at any dosage up to 10 mg/mL.  
**Metabolic activation** : no data  
**Result** : negative  
**Method** : EPA OTS 798.5500  
**Year** : 1991  
**GLP** : yes  
**Test substance** : other TS: >99.96% TRIS NITRO  
**Reliability** : (1) valid without restriction  
14.11.2003

(32)

**Type** : Mouse lymphoma assay  
**System of testing** : Forward mutation of the TK+/- strain of L5178Y mouse lymphoma cells exposed to various concentrations of the test substance.  
**Concentration** : 5 to 80 micrograms/mL without S9 and 5 to 160 micrograms/mL with S9  
**Cycotoxic conc.** : 47.2 micrograms/mL without S9 and 188.8 micrograms/mL with S9  
**Metabolic activation** : with and without

## 5. Toxicity

Id 126-11-4  
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**Result** : positive  
**Method** : OECD Guide-line 476 "Genetic Toxicology: In vitro Mammalian Cell Gene Mutation Tests"  
**Year** : 2002  
**GLP** : yes  
**Test substance** : other TS: 99.69% pure  
**Reliability** : (1) valid without restriction  
20.06.2002 (33)  
20.07.2001

### 5.6 GENETIC TOXICITY 'IN VIVO'

**Type** : Unscheduled DNA synthesis  
**Species** : rat  
**Sex** : male/female  
**Strain** : Fischer 344  
**Route of admin.** : gavage  
**Exposure period** : 2 to 4 or 14 to 16 hours after dosing  
**Doses** : 800 to 1200 mg/kg bw in water  
**Result** : negative  
**Method** : other: OECD Guideline 486  
**Year** : 2002  
**GLP** : yes  
**Test substance** : other TS:99.69% pure TRIS NITRO  
**Reliability** : (1) valid without restriction  
14.11.2003 (34)

**Type** : Micronucleus assay  
**Species** : mouse  
**Sex** : male/female  
**Strain** : CD-1  
**Route of admin.** : gavage  
**Exposure period** : single gavage doses were given on two consecutive days and animals were sacrificed 24 hours after the second dose  
**Doses** : 0, 500, 1000, and 2000 mg/kg bw for males and 0, 500, 1000, and 1500 mg/kg bw for females  
**Result** : negative  
**Method** : OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"  
**Year** : 2002  
**GLP** : yes  
**Test substance** : other TS: 99.69% pure TRIS NITRO  
**Reliability** : (1) valid without restriction  
14.11.2003 (35)

### 5.7 CARCINOGENITY

**Species** :  
**Sex** :  
**Strain** :  
**Route of admin.** :  
**Exposure period** :  
**Frequency of treatment** :  
**Post. obs. period** :  
**Doses** :  
**Result** :  
**Control group** :

Method :  
Year :  
GLP :  
Test substance : no data  
11.06.2001

## 5.8 TOXICITY TO REPRODUCTION

Type : other  
Species : rat  
Sex : male/female  
Strain :  
Route of admin. : dermal  
Exposure period : Six hours per day, Five days per week, for 13 weeks  
Frequency of treatment : Daily except weekends  
Premating exposure period :  
Male : not applicable  
Female : not applicable  
Duration of test : Thirteen weeks  
Doses : 0, 250, 500, and 1000 mg/kg/day  
Control group : yes, concurrent vehicle  
Method : other (calculated)  
Year : 1989  
GLP : yes  
Test substance : other TS: 99.69% pure TRIS NITRO  
Method : An area of approximately 20-25% of the surface area of the rats was clipped free of hair 24 hours before the first application to the skin. The test material was applied as a paste wet with water (0.05, 0.1, and 0.2 mL for the 250, 500, and 1000 mg/kg/day groups respectively). The test material was spread over 6% of the body area with the 250 mg/kg group and over 9% of the body area with the 500 and 1000 mg/kg groups. The control group received deionized water spread over 9-10% of the body area. Animals were dosed daily and the exposed areas covered with a gauze binder secured with tape. After six hours the gauze was removed and the exposed areas washed. All rats wore Elizabethan collars to prevent ingestion of the test material.

Animals were inspected at least twice daily for mortality and overt signs of toxicity. Individual body weights and food consumption were measured weekly beginning one week before initiation of dosing. Ophthalmological examinations were conducted and hematology and clinical chemistry were checked prior to initiation of dosing and just prior to terminal sacrifice. Urinalysis was conducted on all rats during week 12 of the study. All animals were subject to gross and microscopic pathological examination at termination of the study.

Remark : Reproductive Toxicity:  
Males - At sacrifice, there was no significant difference in the weight of the testes of the high dose rats in comparison to the weight of the testes of the controls; neither was there significant difference in their relative weight versus body weight. Histopathologic findings for all animals examined (i.e. controls and high dose rats) were that the testes of all animals were "within normal limits".

Females - Again, the weights (absolute and relative) of the ovaries of all animals were not significantly different. The only histopathologic finding was a minimal cyst in the ovary of one high-dose rat.

Result : The only mortality during the course of the study was for one control female which died in week 4. This death was attributed to an injury sustained

several weeks prior to death.

No clinical signs of toxicity were observed. Although the application sites were discolored yellow throughout the study, microscopic examination of skin samples from the control and high dose group animals did not reveal any adverse effects related to exposure. The test material was essentially nonirritating. No compound related adverse effects were noted on body weights or body weight gain, food consumption, hematology or serum chemistry parameters, urinalysis parameters, absolute or relative organ weights, ophthalmoscopic findings, lesions at gross necropsy, or nonneoplastic histologic lesions

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

(29)

### 5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

**Species** : rat  
**Sex** : female  
**Strain** : Sprague-Dawley  
**Route of admin.** : gavage  
**Exposure period** : Days 6 through 15 of the gestation period.  
**Frequency of treatment** : Single dose daily.  
**Duration of test** :  
**Doses** : 0, 50, 375, and 750 mg/kg/day in 10 mL/kg of water  
**Control group** : yes, concurrent vehicle  
**NOAEL Maternal** : = 375 mg/kg bw  
**NOAEL Teratogen** : = 50 mg/kg bw  
**LOAEL Maternal** : = 750 mg/kg bw  
**Toxicity**  
**LOAEL Teratogenicity** : = 375 mg/kg bw  
**Method** : EPA OPP 83-3  
**Year** : 1989  
**GLP** : yes  
**Test substance** : other TS: 99.69% pure TRIS NITRO  
**Method** : For each test group, twenty-five females were mated 1:1 with males of the same strain and source. The presence of a copulatory plug was positive evidence of mating, and the day it was found was designated day 0 of gestation.

TRIS NITRO for all doses was dissolved in water of a volume of 10 mL/kg bw/day and administered by gavage based on the most recent recorded body weight. Dosing was conducted on days 6 through 15 of gestation. Dosing solutions were analyzed to confirm concentrations.

The dams were checked for mortality and clinical signs of toxicity at least twice a day. Maternal body weights were recorded days 0, 6, 9, 12, 16, and 20 of gestation. On day 20 of gestation, all surviving dams were sacrificed, and litters were delivered by cesarean section.

The females were examined for a number of parameters related to pregnancy including the number corpora lutea, live and dead fetuses, and early and late resorptions. The fetuses were weighed and sexed and examined for external abnormalities. Visceral abnormalities from one-half of the fetuses were determined and skeletal abnormalities were determined for the other half of the litters.

**Result** : Maternal Toxicity:  
High mortality (7 of 25 dams died between days 9 and 11 of gestation), reduced body weight gain during dosing, and clinical signs (e.g. tremors and head bobbing) were observed at 750 mg/kg/day. Similar effects were not observed at lower doses.

**Developmental Toxicity:**

**External Examinations:** One fetus from the low-dose group had an umbilical herniation. Two fetuses from one high-dose litter had omphalocele, and a third fetus from the same litter had an umbilical herniation. Microphthalmia (right eye) was observed in one fetus from the low-dose group.

**Visceral Examinations:** One fetus from the high-dose group had unascended kidneys. Distended ureters and/or undeveloped renal papillae were observed in three fetuses from two control litters and two fetuses from one mid-dose litter.

**Skeletal Examinations:** No skeletal malformations were found in control or test groups. The incidences of skeletal variations such as unossified sternbrae and extra ribs were similar among control and test groups and within the range of historical controls.

**Deaths/resorptions:** A significant, compound related, increase in the number of resorptions/dam was observed at 375 mg/kg/day. This is considered to be a compound-related effect because 1) a nonsignificant increase was also observed at 750 mg/kg/day, 2) the number was above that of historical controls, and 3) had more dams survived the high-dose treatment, the deaths/resorptions would most likely have increased significantly. The toxicity observed at the high-dose level possibly masked the effect slightly. No fetal mortality was observed.

**Altered growth:** A statistically significant reduction in fetal body weight was observed at 750 mg/kg/day.

**Developmental Anomalies -** A nonsignificant increase in the incidence of 7th cervical rib was observed at 375 mg/kg/day. This was slightly above historical control ranges, but because the number of fetuses affected was so small, the increase was not considered to be biologically significant. All other observations were within the range of historical findings.

**Malformations:** A nonsignificant increase in the incidence of omphalocele was observed at 750 mg/kg/day. All other observed incidences were within the range of historical controls. Therefore, the test material was not teratogenic in rats.

**Reliability**  
14.11.2003

: (1) valid without restriction

(36)

**Species**  
**Sex**  
**Strain**  
**Route of admin.**  
**Exposure period**  
**Frequency of treatment**  
**Duration of test**  
**Doses**  
**Control group**  
**NOAEL Maternalt.**  
**NOAEL Teratogen**  
**Method**  
**Year**  
**GLP**  
**Test substance**  
**Method**

: rabbit  
: female  
: New Zealand white  
: gavage  
: Days 7 through 19 of gestation.  
: Once each day of the exposure period.  
: Twenty-nine days  
: 10, 30, and 75 mg/kg/day in a volume of 1 mL/kg bw.  
: yes, concurrent vehicle  
: = 30 mg/kg bw  
: = 75 mg/kg bw  
: EPA OPP 83-3  
: 1992  
: yes  
: other TS: 99.69% pure TRIS NITRO  
: Three groups of twenty artificially inseminated New Zealand white Rabbits were dosed by gavage once daily with 1 mL/kg bw of deionized water containing TRIS NITRO at levels of 10, 30, and 75 mg/kg bw. Dosing was

conducted on days 7 through 19 of gestation. A concurrent control group of 20 rabbits received water only. All females were observed at least twice daily for mortality, appearance, and behavior. Body weights were recorded at appropriate intervals and food consumption was recorded daily (gestation days 0-29). On gestation day 29 the rabbits were euthanized and subjected to Cesarean section. Mean gravid uterine weights and net body weight changes were calculated for each group. The fetuses were weighed, sexed, and examined for external, skeletal, soft tissue malformations, and developmental variations.

**Result**

: Maternal Toxicity:

Mortality: No mortality was observed.

Abortion: No compound-related abortions were observed. One doe at 10 mg/kg/day aborted on GD 29; necropsy revealed accentuation of the lobular markings of the liver, multiple white foci on the gallbladder, reddened cortico-medullary junctions in the kidneys and dark red areas on the glandular portion of the stomach. A second doe at 75 mg/kg/day aborted on Gd 28; necropsy did not reveal cause of death.

Clinical Observations: No compound-related signs were observed. Frequently occurring signs included hair loss, clear nasal discharge, and decreased defecation. These signs were noted at similar incidences for all dose groups.

Body weight and Food Consumption: At a dose level of 75 mg/kg/day, a group mean body weight loss was observed during gestation days 7-10 (statistically significant at  $p < 0.05$ ) and mean body weight gain was inhibited during the overall treatment period (gestation days 7-19). In this same group, food consumption was inhibited throughout the treatment period. Body weight gain and food consumption were not adversely affected in the 10 and 30 mg/kg/day groups.

Developmental Toxicity:

Dose levels (mg/kg/dy)	0	10	30	75
Fetuses (litters)	110(17)	137(17)	139(17)	134(18)

External Malformations

Narrow pelvic reg.	4(1)	0	0	0
Hindlegs hyperextended	2(1)	0	0	0
Carpal &/or tarsal flex.	3(1)	0	0	0
Omphalocele	1	0	0	1
Filamentous tail	0	0	0	1
Totals	6(2)	0	0	2(2)

Visceral Malformations

Bulbous aorta	0	0	3(1)	0
Heart &/or grt. ves. anom	2(2)	0	1	2(2)
Iris bombe	0	0	0	1
Hydrocephaly	1	0	0	0
Totals	3(3)	0	4(1)	3(3)

Skeletal Malformations

Extra ossif. site				
anterior to stern. #1	3(2)	1	1	3(3)
Fused sternebrae	1	1	0	0

## 5. Toxicity

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Only 5 sternebrae	1	0	0	0
Vertebral anomaly with or wo rib anomaly	3(2)	0	0	2(2)
Malaligned sternebrae	0	0	0	1
Totals	8(6)	2(2)	1	6(5)

Totals, fetuses(litters)  
all malformations 14(7) 2(2) 5(2) 9(7)

Developmental toxicity was not observed in this study.

**Reliability** : (1) valid without restriction (37)  
14.11.2003

**Species** : rat  
**Sex** : female  
**Strain** : Sprague-Dawley  
**Route of admin.** : gavage  
**Exposure period** : Days 6 through 15 of gestation  
**Frequency of treatment** : once daily  
**Duration of test** :  
**Doses** : 250, 500, 750, 1000, and 1500 mg/kg/day  
**Control group** : yes, concurrent vehicle  
**NOAEL Maternalt.** : = 500 mg/kg bw  
**NOAEL Teratogen** : = 750 mg/kg bw  
**Method** : EPA OPP 83-3  
**Year** : 1988  
**GLP** : yes  
**Test substance** : other TS: 99.69% pure TRIS NITRO  
**Method** : Five groups of five bred rats were used at each dose in this range-finding study.  
**Result** : One dam died in the 1000 mg/kg group and 3 dams died in the 1500 mg/kg group during treatment. Decreased body weight was observed at the 750 mg/kg dose. No indication of prenatal toxicity was apparent upon evaluation of the gestation day 20 uterine examination data.

**Reliability** : (1) valid without restriction (38)  
14.11.2003

**Species** : rabbit  
**Sex** : female  
**Strain** : New Zealand white  
**Route of admin.** : gavage  
**Exposure period** : days 7 through 19 of gestation  
**Frequency of treatment** : daily during gestation  
**Duration of test** :  
**Doses** : 5, 10, 20, 40, and 80 mg/kg/day  
**Control group** : yes, concurrent vehicle  
**NOAEL Maternalt.** : = 40 mg/kg bw  
**NOAEL Teratogen** : = 80 mg/kg bw  
**Method** : EPA OPP 83-3  
**Year** : 1992  
**GLP** : yes  
**Test substance** : other TS: 99.69% pure TRIS NITRO  
**Method** : Six groups of seven artificially inseminated rabbits were used at each dose.  
**Result** : No dams died in any of the groups. Maternal body weight gain and food consumption were depressed at the 80 mg/kg/day dose level. No effects on the intrauterine growth and survival were observed at any dose level. Neither were any external malformations or variations noted in fetuses.

**Reliability** : (1) valid without restriction (39)  
14.11.2003

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**5.10 OTHER RELEVANT INFORMATION**

**5.11 EXPERIENCE WITH HUMAN EXPOSURE**

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- (18) Bodden, M., (June 28, 1978), "8-Day Dietary Study in the Bobwhite Quail", Raltech Scientific Services RT No. 8032836.
- (19) Parekh, C., (19 June 1979), "LD50 and Eye Irritation of TRIS NITRO Concentrate (P-2350)", IMC Toxicity Laboratory PLR-77.

## 6. References

Id 126-11-4  
Date 10.12.2003

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- (39) Nemeč, M.D., (April 16, 1992), "A Range-Finding Developmental Toxicity Study of TRIS NITRO in Rats", WIL Research Laboratory Report WIL-129007.

## 6. References

**Id** 126-11-4  
**Date** 10.12.2003

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7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

7.3 RISK ASSESSMENT

201-15095B2

# I U C L I D

## Data Set

RECEIVED  
OPPT/CRIC  
04 FEB 12 AM 10:39

**Existing Chemical** : ID: 76-39-1  
**CAS No.** : 76-39-1  
**TSCA Name** : 2-methyl-2-nitro-1-propanol  
**EINECS No.** : 200-957-6

**Producer Related Part**  
**Company** : The Dow Chemical Company  
**Creation date** : 09.08.2001

**Substance Related Part**  
**Company** : The Dow Chemical Company  
**Creation date** : 09.08.2001

**Memo** :

**Printing date** : 14.01.2004  
**Revision date** :  
**Date of last Update** : 09.12.2003

**Number of Pages** : 16

**Chapter (profile)** :  
**Reliability (profile)** :  
**Flags (profile)** : ???

## 1.0.1 OECD AND COMPANY INFORMATION

Type : cooperating company  
Name : The Dow Chemical company  
Partner :  
Date :  
Street : 2020 Dow Center  
Town : 48674 Midland, Michigan  
Country : United States  
Phone :  
Telefax :  
Telex :  
Cedex :  
Reliability : (1) valid without restriction  
14.08.2001

## 1.0.2 LOCATION OF PRODUCTION SITE

Name of Plant : Angus Chemical Company  
Street : Louisiana Highway 2  
Town : 71280 Sterlington, LA  
Country : United States  
Phone :  
Telefax :  
Telex :  
Cedex :  
14.08.2001

## 1.0.3 IDENTITY OF RECIPIENTS

## 1.1 GENERAL SUBSTANCE INFORMATION

Substance type : organic  
Physical status : solid  
Purity : > 99 % w/w  
Remark : This substance, when isolated is solid and crystalline at normal ambient temperatures. It is not, however, normally isolated but is used in an aqueous solution for synthesis on a site limited basis.  
Reliability : (1) valid without restriction  
09.08.2001

### 1.1.0 DETAILS ON TEMPLATE

Comment : One of two HPV chemicals which are defined as the category, nitro alcohols.  
07.12.2001

### 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

**Type** : industrial  
**Category** : Chemical industry: used in synthesis  
**Remark** : Virtually all of this substance being manufactured today is used as a site limited intermediate for the synthesis of 2 -amino-2-methyl-1-propanol.  
**Reliability** : (1) valid without restriction  
14.08.2001

## 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. General Information

Id 76-39-1  
Date 15.12.2003

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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** : = 90 °C  
**Remark** : At ambient pressure, decomposition begins at temperatures slightly above the melting point.  
**Reliability** : (2) valid with restrictions  
31.10.2003 (1)

### 2.2 BOILING POINT

**Value** : = 94 °C at 19.5 hPa  
**Reliability** : (2) valid with restrictions  
14.08.2001 (1)

### 2.3 DENSITY

#### 2.3.1 GRANULOMETRY

### 2.4 VAPOUR PRESSURE

**Remark** : 2-Methyl-2-nitro-1-propanol is essentially nonvolatile. Its vapor pressure at 94 degrees centigrade is only 19.5 hPa. Even this pressure may be the off-gassing of formaldehyde due to decomposition of the molecule.  
**Reliability** : (2) valid with restrictions  
26.11.2002 (2)

### 2.5 PARTITION COEFFICIENT

#### 2.6.1 WATER SOLUBILITY

**Value** : = 350 other: g per 100 mL water at 25 °C  
**Qualitative** :  
**Pka** : at 25 °C  
**PH** : at and °C  
**Reliability** : (2) valid with restrictions  
22.10.2002 (1)

#### 2.6.2 SURFACE TENSION

**Remark** : Not applicable to this solid material.  
**Reliability** : (1) valid without restriction  
14.08.2001

### 2.7 FLASH POINT

**Remark** : Not applicable to this solid material.  
**Reliability** : (1) valid without restriction

## 2. Physico-Chemical Data

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### 2.8 AUTO FLAMMABILITY

**Remark** : Not applicable to this solid material.  
**Reliability** : (2) valid with restrictions  
14.08.2001

### 2.9 FLAMMABILITY

### 2.10 EXPLOSIVE PROPERTIES

### 2.11 OXIDIZING PROPERTIES

### 2.12 ADDITIONAL REMARKS

#### 3.1.1 PHOTODEGRADATION

**Type** : air  
**Light source** :  
**Light spect.** : nm  
**Rel. intensity** : based on Intensity of Sunlight  
**Deg. Product** :  
**Method** : other (calculated): Atmospheric Oxidation Program (AOPWIN)  
**Year** : 2002  
**GLP** : no  
**Test substance** :  
**Method** : The estimated atmospheric half-life based on hydroxyl radical attack was obtained using the AOPWIN version 1.90 computer program assuming 12-hour days.  
**Result** : The atmospheric half-life was estimated to be 14 days.  
27.11.2002

#### 3.1.2 STABILITY IN WATER

**Remark** : While no definitive study has been conducted on this substance it is known, based on experience with tris(hydroxymethyl)nitromethane that the nitro alcohols all hydrolyze at basic pH to yield formaldehyde and nitroparaffins. In the case of 2-methyl-2-nitro-1-propanol the nitroparaffin formed is 2-nitropropane.  
**Reliability** : (1) valid without restriction  
14.08.2001

#### 3.1.3 STABILITY IN SOIL

### 3.2 MONITORING DATA

#### 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

**Type** : fugacity model level I  
**Media** :  
**Air (level I)** :  
**Water (level I)** : 99.9  
**Soil (level I)** : .1  
**Biota (level II / III)** :  
**Soil (level II / III)** : 43.4  
**Method** : other  
**Year** : 2002  
**Remark** : Regardless of the media to which MNP is released, a large majority at steady state is in the soil and water phases.  
**Result** : Using the default emissions of equal amounts to soil, air, water and sediment (1000 kg/hr for each) the Level III model predicts that the distribution of MNP will be 43.4% in soil, 39.4% in water, 17.1 % in sediment, and <0.1% in air.  
13.12.2002

(3)

#### 3.3.2 DISTRIBUTION

#### 3.4 MODE OF DEGRADATION IN ACTUAL USE

#### 3.5 BIODEGRADATION

**Remark** : Based upon the result of the biodegradation study of 2-(hydroxymethyl)-2-nitro-1,3-propanediol, this substance is not readily biodegradable.  
**Reliability** : (1) valid without restriction  
31.10.2003

#### 3.6 BOD5, COD OR BOD5/COD RATIO

#### 3.7 BIOACCUMULATION

#### 3.8 ADDITIONAL REMARKS

## 4.1 ACUTE/PROLONGED TOXICITY TO FISH

**Type** : other: predicted value  
**Species** :  
**Exposure period** :  
**Unit** :  
**Analytical monitoring** :  
**Method** :  
**Year** :  
**GLP** :  
**Test substance** : as prescribed by 1.1 - 1.4  
**Remark** : This program only examines the toxicity of the parent compound and would not examine potential break down products such as formaldehyde.  
**Result** : The ECOSAR v0.99g program using the Neutral Organics Class and default parameters of Log Kow = -0.14 and Water Solubility = 80680 mg/L was used to predict fish toxicity. The predicted 96-hour LC50 for fish was 9070 mg/L.  
**Reliability** : (2) valid with restrictions  
 2F  
 14.01.2004

## 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

**Type** : other: predicted value  
**Species** :  
**Exposure period** :  
**Unit** :  
**Analytical monitoring** :  
**Method** :  
**Year** :  
**GLP** :  
**Test substance** : as prescribed by 1.1 - 1.4  
**Remark** : This program only examines the toxicity of the parent compound and would not examine potential break down products such as formaldehyde.  
**Result** : The ECOSAR v0.99g program using the Neutral Organics Class and default parameters of Log Kow = -0.14 and Water Solubility = 80680 mg/L was used to predict daphnia toxicity. The predicted 48-hour LC50 for daphnia was 8383 mg/L.  
**Reliability** : (2) valid with restrictions                      2F  
 2F  
 14.01.2004

## 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

**Species** :  
**Endpoint** : other: predicted value  
**Exposure period** :  
**Unit** :  
**Analytical monitoring** :  
**Method** :  
**Year** :  
**GLP** :  
**Test substance** : as prescribed by 1.1 - 1.4  
**Remark** : This program only examines the toxicity of the parent compound and would not examine potential break down products such as formaldehyde.  
**Result** : The ECOSAR v0.99g program using the Neutral Organics Class and

Reliability : default parameters of Log Kow = -0.14 and Water Solubility = 80680 mg/L was used to predict algae toxicity. The predicted 96-hour EC50 for algae was 4633 mg/L.  
: (2) valid with restrictions  
2F  
14.01.2004

### 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 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

## 5.1.1 ACUTE ORAL TOXICITY

<b>Type</b>	:	LD50
<b>Species</b>	:	rat
<b>Strain</b>	:	other: Cox-SD
<b>Sex</b>	:	male/female
<b>Number of animals</b>	:	130
<b>Vehicle</b>	:	water
<b>Value</b>	:	= 845 - 1480 mg/kg bw
<b>Method</b>	:	other: IMC Toxicity Laboratory Protocol
<b>Year</b>	:	1980
<b>GLP</b>	:	no
<b>Test substance</b>	:	other TS: 99.6 % pure
<b>Method</b>	:	Cox-SD albino rats weighing 200 +/-25 g were dosed by gavage with test material in sterile deionized water. Groups of ten males were dosed at 0, 402, 570, 800, 1100, 1600, and 2300 mg/kg bw. Groups of ten females were dosed at 0, 800, 1100, 1310, 1600, and 2300 mg/kg bw. All animals were observed frequently on the day of compound administration and at least once a day thereafter for 14 days. All animals that died during this period were necropsied on the day of death or the day after death for rats that died overnight. After 14 days all surviving rats were weighed, sacrificed, and examined for gross pathology.
<b>Result</b>	:	Male rats exhibited signs of toxicity at all dose levels. At 800 mg/kg, the rats were lethargic and ataxic 30 minutes after dosing. At higher doses, the rats were prostrate and breathing slowly after 30 minutes. One rat each in the 800, 1100, and 1600 mg/kg groups showed mottled livers at necropsy. Female rats were more resistant to the compound and showed fewer signs of toxicity. With the 1600mg/kg group only, the rats were prostrate 24 hours after dosing and 7/10 exhibited mild hematuria. At necropsy, all organs were grossly normal. Deaths in all groups occurred within the first three days following dosing. The LD50 for males was calculated to be 845 (710-1150) mg/kg. For females the LD50 was 1480 (1370- 1598) mg/kg.
<b>Reliability</b>	:	(2) valid with restrictions
26.11.2002		(4)

## 5.1.2 ACUTE INHALATION TOXICITY

## 5.1.3 ACUTE DERMAL TOXICITY

<b>Type</b>	:	other: Dermal toxicity limit test
<b>Species</b>	:	rabbit
<b>Strain</b>	:	New Zealand white
<b>Sex</b>	:	male/female
<b>Number of animals</b>	:	10
<b>Vehicle</b>	:	water
<b>Value</b>	:	> 2000 mg/kg bw
<b>Method</b>	:	other: IMC Toxicity Laboratory Protocol
<b>Year</b>	:	1980
<b>GLP</b>	:	no
<b>Test substance</b>	:	other TS: 99.6 % pure
<b>Method</b>	:	Ten New Zealand White rabbits weighing 2.9 +/-0.5 kg were placed in two groups. The abdomens of the rabbits were shaved free of hair. The abdomens of 3 males and 2 females were abraded without bleeding with a blunt hypodermic needle. All animals then were treated with 2000 mg/kg

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bw of the test compound which dissolved readily in moisture present on the skin. The exposed skin was covered with gauze and impervious rubber cloth. After 24 hours, this cover was removed and the exposed skin was evaluated for irritancy. The rabbits were then observed for 14 days prior to sacrifice and pathological examination.

**Result** : No rabbits died during the test period and no signs of toxicity were observed. There was no irritation of the skin, and at necropsy, all organs examined were grossly normal.

**Reliability** : (2) valid with restrictions  
07.12.2001 (4)

### 5.1.4 ACUTE TOXICITY, OTHER ROUTES

#### 5.2.1 SKIN IRRITATION

**Species** : rabbit  
**Concentration** : undiluted  
**Exposure** : Occlusive  
**Exposure time** : 24 hour(s)  
**Number of animals** : 6  
**PDII** : .13  
**Result** : not irritating  
**EC classification** : not irritating  
**Method** : other: IMC Toxicology Laboratory Protocol  
**Year** : 1980  
**GLP** : no  
**Test substance** : other TS: 99.6 % pure  
**Method** : The backs of 6 New Zealand White rabbits weighing 3.0 +/- 0.5 kg were clipped free of hair. The skin area on the left side of the mid dorsal line was left intact while that to the right was abraded in a tic-tac-toe pattern with a blunt hypodermic needle. Both sides of the backs of the animals received 0.5 g of test compound which readily dissolved in the moisture present on the skin. The animals backs were then covered with a gauze pad and occlusive cloth for 24 hours. After exposure, the treated sites were cleaned and scored for skin reaction. They were also scored at 72 hours (48 hours after the first scoring).

**Result** : Only three rabbits (one at the abraded site) exhibited minimal erythema at 24 hours. No irritation was observed at 72 hours. The primary irritation index was 0.13.

**Reliability** : (2) valid with restrictions  
10.08.2001 (4)

#### 5.2.2 EYE IRRITATION

**Species** : rabbit  
**Concentration** : undiluted  
**Dose** : .1 other: gram  
**Exposure Time** : 24 hour(s)  
**Comment** : not rinsed  
**Number of animals** : 6  
**Result** : highly irritating  
**EC classification** : risk of serious damage to eyes  
**Method** : other: IMC Toxicology Laboratory Protocol  
**Year** : 1980  
**GLP** : no  
**Test substance** : other TS: 99.6 % pure  
**Method** : The test compound was ground to a fine powder and 0.1 g was instilled

into the lower conjunctival sac of the right eye of each of 6 New Zealand White rabbits. The eye was held closed for two seconds to prevent loss of material. The eyes were then examined at 24, 48, and 72 hours post treatment. At 72 hours and on the 7th day, a drop of sodium fluorescein (0.24%) was placed in the eye and the excess washed from the eye with sterile saline. The eyes were then examined under UV light for corneal lesions.

**Result** : The compound affected the cornea, iris, and conjunctiva of all rabbits. At 72 hours, the eyes of all 6 rabbits showed corneal scarring. When re-examined after 7 days, very little if any recovery was evident. The average score for the study ranged from 36.5-37.7. The compound is a severe eye irritant.

**Reliability** : (2) valid with restrictions  
07.12.2001 (4)

**5.3 SENSITIZATION**

**Type** : Buehler Test  
**Species** : guinea pig  
**Concentration** : Induction 25 % active substance occlusive epicutaneous  
Challenge 25 % active substance occlusive epicutaneous

**Number of animals** : 30  
**Vehicle** : water  
**Result** : not sensitizing  
**Classification** : not sensitizing  
**Method** : other: IMC Toxicology Laboratory protocol  
**Year** : 1980  
**GLP** : no  
**Test substance** : other TS: 99.6 % pure  
**Method** : The backs and flanks of 30 female guinea pigs weighing 250-300 g were shaved free of hair. One group of ten animals was treated topically with 0.5 mL of 25 % test compound. A second group was treated with 0.5 mL of 5% formaldehyde, and a third group received 0.5 mL of 1% carboxymethyl cellulose (CMC) in water. After 24 hours under occlusive cover the sites were cleaned. This procedure was repeated once a week for three weeks after which the animals were allowed to rest for two weeks. On the first day of the third week each group of animals was challenged topically as follows:  
Group 1 received 5, 10, and 25% test compound  
Group 2 received 2% formaldehyde  
Group 3 received all the above as well as 1% CMC

**Result** : Only 6 of the 10 animals in Group 2 reacted. All other animals did not react.

**Reliability** : (2) valid with restrictions  
07.12.2001 (4)

**5.4 REPEATED DOSE TOXICITY****5.5 GENETIC TOXICITY 'IN VITRO'**

**Type** : Ames test  
**System of testing** : Tested in Salmonella typhimurium strains TA98, TA100, TA1537, and TA1538.  
**Concentration** : 0, 0.1, 0.5, 2.5, 5.0, and 10 micro liter/plate  
**Cycotoxic conc.** : There was no significant effect of the test substance on viability of the bacteria.

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**Metabolic activation** : with and without  
**Result** : negative  
**Method** : other: EG&G Mason Protocol  
**Year** : 1980  
**GLP** : no  
**Test substance** : other TS: 60.1% active in MeOH/water  
**Method** : The toxicity of MNP, the test article, was determined using TA100 and MNP at concentrations of 0.003 micro grams per plate up to 10 micro grams per plate. No significant difference was noted at any concentration in comparison to water in terms of viable cell count/plate, revertants/plate, or background bacterial lawn. No precipitation of the test article was observed.

The positive controls utilized were as follows:

For TA98 1.0 microgram 2-aminoanthracene

For TA98 10.0 microgram 2-nitrofluorene

For TA100 1.0 microgram 2-aminoanthracene

For TA1535 0.04 microgram 1,3-propane sultone

For TA1537 0.04 microgram 1,3-propane sultone

For TA1538 10.0 microgram 2-nitrofluorene

All positive controls elicited the expected positive result.

All concentrations of the test article, the positive controls, and the solvent(water) control were plated in triplicate and incubated at 37 degrees C for 48 hours before evaluation. The test article and solvent control were tested with and without S9 rat liver microsomal enzyme.

**Result** : None of the test plates met the criterion for a positive response (a doubling of the revertants when compared with the solvent control). In most cases the high concentration plate was essentially no different from the control in terms of the number of revertants.

**Reliability** : (2) valid with restrictions  
09.12.2003

(5)

### 5.6 GENETIC TOXICITY 'IN VIVO'

### 5.7 CARCINOGENITY

### 5.8 TOXICITY TO REPRODUCTION

### 5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

### 5.10 OTHER RELEVANT INFORMATION

### 5.11 EXPERIENCE WITH HUMAN EXPOSURE

## 6. References

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**7.1 END POINT SUMMARY**

**7.2 HAZARD SUMMARY**

**7.3 RISK ASSESSMENT**