FOREWORD

NEOPENTYL GLYCOL
CAS N°: 126-30-7

INTRODUCTION
Substance

End Point : IDENTIFIERS, PHYSICAL AND CHEMICAL PROPERTIES
Chemical Name : 1,3-Propanediol, 2,2-dimethyl
Common Name : Neopentyl glycol
CAS Number : 126-30-7
RTECS Number : TY5775000

Synonyms

2,2-Dimethyl-1,3-propanediol
Neopentyl glycol

Dimethyltrimethylene glycol

Properties & Definitions

Molecular Formula : C5H12O2
Molecular Weight : 104.15
Melting Point : 127°C
Boiling Point : 208°C
Vapour Pressure : 30 mmHg (140°C), 760 mmHg (211°C)
Octanol/Water Partition Coefficient : log Pow = 0.12 at 25°C (measured)
Water Solubility : 190g/100 ml at 20°C (65%)
Impurities : Neopentyl glycol formic acid ester and neopentyl glycol isolactic acid ester
General Comments : Thermal decomposition occurs at higher than 120°C in strong base. Thermal decomposition products: methanol, isobutanol, isobutyl aldehyde, formaldehyde etc.

Overall Evaluation

SIDS INITIAL ASSESSMENT

This substance is presently of low priority for further work.

SHORT SUMMARY OF THE REASONS WHICH SUPPORT THE RECOMMENDATION:

2,2-Dimethyl-1,3-propanediol is stable solid, and the production volume is 12,000 tonnes for 1991 in Japan. This chemical is stable in neutral, acidic or alkaline solutions, and is classified as "not readily biodegradable" by the results of the biodegradation test conducted as SIDS testing. The chemical is non-toxic to fish, daphnids and algae. The chemical showed no genotoxic effects, and NOAEL for repeated dose toxicity was 100 mg/kg/day and NOAEL for reproductive toxicity was 1000 mg/kg/day. Estimated dose of low concern (EDCL) was calculated as 0.1 mg/kg/day and 10.0 mg/kg/day for repeated dose toxicity and reproductive toxicity, respectively. Daily intake of the chemical was estimated as 1.11E mg/day from calculation using MNSEM 145J exposure model. In conclusion, although 2,2-dimethyl-1,3-propanediol is persistent and toxicological test showed moderate toxicity, no further testing is needed at present considering its exposure levels.

However, international information on exposure is needed for consideration of more realistic analysis.
Production-Trade

Chemical Name : 1,3-Propanediol, 2,2-dimethyl
CAS Number : 126-30-7
Geographic Area : JPN

Production

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Year</th>
</tr>
</thead>
<tbody>
<tr>
<td>14000 T/Y - P</td>
<td>1985</td>
</tr>
<tr>
<td>12000 T/Y - P</td>
<td>1991</td>
</tr>
<tr>
<td>4000 T/Y - IM</td>
<td>1991</td>
</tr>
</tbody>
</table>

References

!SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)
Uses

Chemical Name : 1,3-Propanediol, 2,2-dimethyl-
CAS Number : 126-30-7
Geographic Area : JPN

Use

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Year</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>7300 T</td>
<td></td>
<td>Raw material for alkid resins</td>
</tr>
<tr>
<td>5900 T</td>
<td></td>
<td>Raw material for unsaturated polyester resins</td>
</tr>
<tr>
<td>1800 T</td>
<td></td>
<td>Raw material for powder paint resin</td>
</tr>
<tr>
<td>1000 T</td>
<td></td>
<td>Other uses-unspecified</td>
</tr>
</tbody>
</table>

References

Primary References : #MITIR*
                Chemical Report submitted by the Ministry of International Trade and Industry, Japan

Secondary References : !SIDSP*
            OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)
Study

End Point : CONCENTRATION
Chemical Name : 1,3-Propanediol, 2,2-dimethyl
CAS Number : 126-30-7
Study type : MODEL
Geographic Area : JPN

Test Subject

<table>
<thead>
<tr>
<th>Organism</th>
<th>Medium</th>
<th>Specification</th>
<th>Lifestage</th>
<th>Sex</th>
</tr>
</thead>
<tbody>
<tr>
<td>AIR</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>AQ</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SOIL</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Test Method and Conditions

Test method : Multi-phase, non-steady state equilibrium model (MNSEM 145J) for evaluation of fate of chemicals in environment consisting of air, water, soil and sediment phases and food. Version 145J. All values are calculated.

Test Results

<table>
<thead>
<tr>
<th>Matrix</th>
<th>Concentrations</th>
<th>Spec.</th>
<th>Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>AIR</td>
<td>1.79E-10 ppm</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Steady state (SS) mass = 1.53E+0g</td>
<td></td>
<td></td>
</tr>
<tr>
<td>AQ</td>
<td>5.08E-04 mg/l</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>In water SS-mass = 1.02E+07g was also given.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SOIL</td>
<td>3.85E-05 mg/l</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>In soil; a second value of SS-mass = 6.16E+04g was also given.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SED</td>
<td>1.53E-03 mg/l</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>In sediment SS-mass = 1.53E+05g was also given.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>FOOD</td>
<td>2.37E-10 mg/l</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>In meat.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>FOOD</td>
<td>2.24E-10 mg/l</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>In milk.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>PLANT</td>
<td>2.42E-04 mg/l</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>In vegetation.</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
References

Primary Reference : #EAMIT*
MITI ENVIRON. Agency. Exposure Estimation conducted by MITI and Environmental Agency (EA), Japan

Secondary Reference : !SIDSP*
OECD/SDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

Study

End Point : CONCENTRATION
Chemical Name : 1-3 Propanediol, 2,2-dimethyl
CAS Number : 126-30-7
Geographic Area : JPN

Test Subject

<table>
<thead>
<tr>
<th>Organism</th>
<th>Medium</th>
<th>Specification</th>
<th>Lifestage</th>
<th>Sex</th>
</tr>
</thead>
<tbody>
<tr>
<td>AQ</td>
<td>SURF</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SOIL</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SED</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Species/strain/system : Two areas in Japan

Test Results

<table>
<thead>
<tr>
<th>Matrix</th>
<th>Concentrations</th>
<th>Spec.</th>
<th>Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>AQ</td>
<td>ND</td>
<td></td>
<td>1977-</td>
</tr>
</tbody>
</table>
Not detected in surface water. (Detection limit:0.2-0.4mg/l)

SOIL ND 1977-
Not detected in soil or sediment. (Detection limit:0.002mg/l)

References

Primary Reference : #MOREA*
E. A. Environmental Monitoring of Chemicals, Environmental Survey Report (Office of Health Studies, Department of Environmental Health), Japan, (1977)

Secondary Reference : !SIDSP*
OECD/SDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, 6-7, (1993)
### Study

**End Point**: HUMAN INTAKE AND EXPOSURE

**Chemical Name**: 1,3-Propanediol, 2,2-dimethyl

**CAS Number**: 126-30-7

**Geographic Area**: JPN

### Test Subject

<table>
<thead>
<tr>
<th>Organism</th>
<th>Medium</th>
<th>Specification</th>
<th>Route</th>
<th>Lifestage</th>
<th>Sex</th>
</tr>
</thead>
<tbody>
<tr>
<td>FOOD</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Species/strain/system**: Fish, meat, milk and vegetables

### Test Method and Conditions

**Test method description**: Multi-phase, non-steady state equilibrium model (MNSEM 145J) for evaluation of fate of chemicals in environment consisting of air, water, soil and sediment phases. Version 145J (presented by Kikuo Yoshuda). All values are calculated

### Test Results

<table>
<thead>
<tr>
<th>Intake</th>
<th>Spec.</th>
<th>Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.11E-3 mg/d</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.45E-08 mg/d</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.02E-03 mg/d</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.89E-06 mg/d</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.76E-11 mg/d</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.74E-11 mg/d</td>
<td></td>
<td></td>
</tr>
<tr>
<td>9.05E-05 mg/d</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Total exposure dose calculated.

- From inhalation of air.
- From drinking water.
- From ingestion of fish.
- From ingestion of meat.
- From ingestion of milk.
- From ingestion of vegetable.

**General Comments**: Consumer exposure seems to be low because this chemical is used as raw material, and processed in closed system except packaging.

### References

**Secondary Reference**: !SIDSP*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)
Study

End Point : BIODEGRADATION
Chemical Name : 1,3-Propanediol, 2,2-dimethyl
CAS Number : 126-30-7
Study type : LAB
Geographic Area : JPN

Test Subject

Organism Medium Specification

AQ SLUDG

Species/strain/system : Activated sludge 30mg/l as suspended solid

Test Substance

Purity Grade : 99.4%

Test Method and Conditions

Test method description : OECD Guideline 301 C. The sludge samples were mixed by stirring in a single container and then cultured at 25C for 1 month. GLP: yes
Temperature : 25C
(An)aerobic : AEROB

Exposure

Exposure Period : 1 mo
Dose / Concentration : 100 mg/l

Test Results

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Time</th>
<th>Comments on result</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.6 %</td>
<td>LOSS</td>
<td>Degree of biodegradation from BOD 14</td>
</tr>
<tr>
<td>1 %</td>
<td>LOSS</td>
<td>Degree of biodegradation from DOC</td>
</tr>
<tr>
<td>0 %</td>
<td></td>
<td>Degree of biodegradation from GC</td>
</tr>
</tbody>
</table>

Total oxygen demand (TOD) = 64.5 mg

General Comments : These results indicate that neopentyl glycol should be classified as “not readily biodegradable”.

References

Primary Reference : #MITIT*
Test conducted by the Ministry of International Trade and Industry (MITI), Japan

Secondary Reference : !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, 4, (1993)
Study

End Point : PHOTODEGRADATION
Chemical Name : 1,3-Propanediol, 2,2-dimethyl
CAS Number : 126-30-7
Study type : LAB

Test Results

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Time</th>
<th>Comments on result</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Photochemical degradation rate reported as 0.00. T/2 = infinitude.</td>
</tr>
</tbody>
</table>

References

Primary Reference : #MITIT*
Test conducted by the Ministry of International Trade and Industry (MITI), Japan

Secondary Reference : !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)
Study

End Point : HYDROLYSIS
Chemical Name : 1,3-Propanediol, 2,2-dimethyl
CAS Number : 126-30-7
Study type : LAB

Test Substance

Purity Grade : 99.4%

Test Method and Conditions

Temperature : 25 C
pH : 4-9

Test Results

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Time</th>
<th>Comments on result</th>
</tr>
</thead>
<tbody>
<tr>
<td>50 %</td>
<td>1 y</td>
<td>T/2 of test compound in pH 4.0, 7.0 and 9.0 at 25C.</td>
</tr>
</tbody>
</table>

References

Primary Reference : #MITIT*
Test conducted by the Ministry of International Trade and Industry (MITI), Japan, (1993)

Secondary Reference : !SIDSP*
Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)
Study

End Point : BIOCONCENTRATION
Chemical Name : 1,3-Propanediol, 2,2-dimethyl-
CAS Number : 126-30-7

Test Subject

Organism Medium Specification Route Lifestage Sex Number exposed Number controls
FISH

Species/strain/system : Japanese carp*

Test Substance

Description of the test substance : Neopentyl glycol
Purity Grade : >98%

Test Method and Conditions


Exposure

Exposure comments : Level 1 exposure means low exposure level. Level 2 exposure means higher exposure level and is 10x higher in concentration than the low one.

Test Results

Bioconcent. Calc
Organ Factor Basis Time State Comments on result
--------- ------------- --------- -------- ------------------------------
0          ------------  --------  ------- log BCF for level 1 exposure.

1          ------------  --------  ------- log BCF for level 2 exposure.

General Comments : * Specific details on the lifestage of the test organism and test conditions were not given.

References

Primary Reference : #MITIT*
Test conducted by the Ministry of International Trade and Industry (MITI), Japan

Secondary Reference : ISIDSP* Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)
### Study

- **End Point**: MAMMALIAN ACUTE TOXICITY
- **Chemical Name**: 1,3-Propanediol, 2,2-dimethyl
- **CAS Number**: 126-30-7

- **Exposure Type**: ACUTE
- **Dose / Concentration**: 3.200 mg/kg

### Test Results

<table>
<thead>
<tr>
<th>Organism</th>
<th>Medium</th>
<th>Spec.</th>
<th>Route</th>
<th>Lifestage</th>
<th>Sex</th>
<th>Effect</th>
<th>Effect Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>RAT</td>
<td>ORL</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>LD50</td>
<td></td>
</tr>
</tbody>
</table>

### References

- **Primary Reference**:
  - #URKOD*
  - Eastman Kodak Company Reports, (1993)

- **Secondary Reference**:
  - !SIDSP*
  - OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

### Study

- **End Point**: MAMMALIAN ACUTE TOXICITY
- **Chemical Name**: 1,3-Propanediol, 2,2-dimethyl
- **CAS Number**: 126-30-7

- **Species/strain/system**: Strain not specified

### Test Results

<table>
<thead>
<tr>
<th>Organism</th>
<th>Medium</th>
<th>Spec.</th>
<th>Route</th>
<th>Lifestage</th>
<th>Sex</th>
<th>Effect</th>
<th>Effect Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>RAT</td>
<td>ORL</td>
<td>ADULT</td>
<td></td>
<td></td>
<td></td>
<td>LD50</td>
<td>Oral acute toxicity dose was reported as 3200mg/kg.</td>
</tr>
</tbody>
</table>

### References

- **Primary Reference**:
  - #URKOD*
  - Eastman Kodak Company Reports, (1971)

- **Secondary Reference**:
  - !SIDSP*
  - OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, 10, (1993)
Study

End Point : MAMMALIAN TOXICITY
Chemical Name : 1,3-Propanediol, 2,2-dimethyl-
CAS Number : 126-30-7

Test Subject

<table>
<thead>
<tr>
<th>Organism</th>
<th>Medium</th>
<th>Specification</th>
<th>Route</th>
<th>Lifestage</th>
<th>Sex</th>
<th>Number exposed</th>
<th>Number controls</th>
</tr>
</thead>
<tbody>
<tr>
<td>RAT</td>
<td>ORL</td>
<td>M</td>
<td>F</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Species/strain/system : Slc: SD strain

Test Substance

Description of the test substance : Neopentyl glycol
Purity Grade : 99.1%
Vehicle - Solvent : Distilled water

Test Method and Conditions

Test method description : OECD Combined Repeated Dose and Reproductive/Developmental Toxicity Screening Test. Killing day: male/day 43; female/day 4 of lactation. GLP: yes.

Exposure

Dose / Concentration : 100-1000 mg/kg /d
Exposure comments : Per gavage to 0 (vehicle), 100, 300, 1000mg/kg/day. Administration period: male: 42 days; female: from 14 day before mating to day 3 of lactation.

Test Results

<table>
<thead>
<tr>
<th>Organ</th>
<th>Effect</th>
<th>Rev.</th>
<th>OnSet</th>
<th>Sex</th>
<th>Affected in Exposed - Controls</th>
</tr>
</thead>
<tbody>
<tr>
<td>NEF</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

There were no dead or no abnormal animals with clinical signs suggested to be relating to the treatment. Bodyweight and food consumption did not reveal consistent or apparently treatment-related differences with the control groups. No observed effects on haematology of the treated male rats.

BLOOD  BIOCH
Blood chemical examination revealed an elevation in values of total protein, total bilirubin and albumin for male rats receiving 300 and 1,000mg/kg. Moreover, glucose values were depressed for male rats receiving 1,000mg/kg.

LIVER  SIZE
KIDNY  SIZE
Absolute and relative weights of the liver and kidney of both male and female rats receiving 300 and 1,000mg/kg were elevated.

LIVER  SIZE
Necropsy revealed hypertrophy of the liver in 2 males receiving 1,000mg/kg. No definite lesion was found histologically. Histopathological examination revealed high incidence of protein casts, hyaline droplet and basophilic change of the renal tubules in males at 1,000mg/kg.

NOAEL
Dose or concentration at which no toxic effects were observed: NOAEL: 100mg/kg/day.

General Comments : Estimated Dose of Low Concern: EDLC = 0.1mg/kg/day.
References

Primary Reference : #URMHW*
Unpublished Report on Combined Repeated Dose and Reproductive/Developmental Toxicity Screening Test conducted by the Ministry of Health and Welfare (MHW), Japan

Secondary Reference : !SIDSP*
Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

Study

End Point : MAMMALIAN TOXICITY
Chemical Name : Neopentyl glycol
CAS Number : 126-30-7
Study type : LAB

Test Subject

<table>
<thead>
<tr>
<th>Organism</th>
<th>Medium</th>
<th>Specification</th>
<th>Route</th>
<th>Lifestage</th>
<th>Sex</th>
<th>Number exposed</th>
<th>Number controls</th>
</tr>
</thead>
<tbody>
<tr>
<td>RAT</td>
<td>ORL</td>
<td>ADULT</td>
<td>M</td>
<td>F</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Species/strain/system : Slc:SD strain

Test Substance

Purity Grade : 99%

Test Method and Conditions

Test method description : OECD Combined Repeated Dose and Reproductive/Developmental Toxicity Screening Test. GLP: yes.

Exposure

Exposure Period : 100-1000 mg
Exposure comments : The doses 0, 100, 300, 1000 mg/kg/day were administered in oral gavage for 42 days to the males and for 14 days before mating to the females and continued through 3-rd day of lactation.
Test Results

<table>
<thead>
<tr>
<th>Organ</th>
<th>Effect</th>
<th>Rev.</th>
<th>OnSet</th>
<th>Sex</th>
<th>Exposed - Controls</th>
</tr>
</thead>
<tbody>
<tr>
<td>BLOOD</td>
<td>BIOCH</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Chemical examination of blood revealed elevated values of: total protein, total bilirubin and albumin for male rats receiving 300 and 1000 mg/kg of neopentyl glycol. The glucose values were depressed for male rats receiving 100 mg/kg of the test substance.

| LIVER  | SIZE   |      |       |     |                    |

Absolute and relative weights of liver and kidneys of both males and females receiving 300 and 1000mg/kg were elevated.

| KIDNY  | SIZE   |      |       |     |                    |

Absolute and relative weights of liver and kidneys of both males and females receiving 300 and 1000mg/kg were elevated.

| LIVER  | STRUC  |      |       |     |                    |

Necropsy revealed hypertrophy of the liver in 2 rats receiving the dose of 1000mg/kg but there was not definite lesions found on microscopic examination.

| KIDNY  | STRUC  |      |       |     |                    |

Histopathological examination revealed high incidence of protein casts, hyaline droplet and basophilic change in renal tubules in male rats on 1000mg/kg dose.

| NOAEL  |        |      |       |     |                    |

Dose of 100mg/kg/day was the dose at which no toxic effects were observed.

| EDCL   |        |      |       |     |                    |

Estimated dose of low concern was calculated as 0.1mg/kg/day.

References

*Primary Reference*: #URMHW

Unpublished Report on Combined Repeated Dose and Reproductive/Developmental Toxicity Screening Test conducted by the Ministry of Health and Welfare (MHW), Japan

*Secondary Reference*: !SIDSP

OECD/SIDS, Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, 11-12, (1993)
Study

End Point : MUTAGENICITY
Chemical Name : 1,3-Propanediol, 2,2-dimethyl-
CAS Number : 126-30-7

Test Subject

Organism Medium Specification Route Lifestage Sex Number exposed Number controls
BACT
Species/strain/system : Salmonella typhimurium /TA100, TA1535, TA98,TA1537; Escherichia coli WP2 uvrA

Test Substance

Description of the test substance : Neopentyl glycol
Purity Grade : 99.1%
Vehicle - Solvent : Distilled water

Test Method and Conditions


Exposure

Exposure comments : The exposure doses used: 0, 312.5, 625, 1250, 2500, 5000ug/plate.

Test Results

<table>
<thead>
<tr>
<th>Organ</th>
<th>Effect</th>
<th>Rev.</th>
<th>OnSet</th>
<th>Sex</th>
<th>Affected in Exposed - Controls</th>
</tr>
</thead>
<tbody>
<tr>
<td>NEF</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The test material was classified as "negative" under the experimental condition used.

General Comments : Minimum concentration of test substance at which toxicity to bacteria was observed: with and without metabolic activation: >5000ug/plate.

References

Primary Reference : #URMMT*

Secondary Reference : !SIDSP*
Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)
Study

End Point: MUTAGENICITY
Chemical Name: 1,3-Propanediol, 2,2-dimethyl-
CAS Number: 126-30-7
Study type: LAB

Test Subject

<table>
<thead>
<tr>
<th>Organism</th>
<th>Medium</th>
<th>Specification</th>
<th>Route</th>
<th>Lifestage</th>
<th>Sex</th>
<th>Number exposed</th>
<th>Number controls</th>
</tr>
</thead>
<tbody>
<tr>
<td>HAMST</td>
<td>VTR</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Species/strain/system: Chinese hamster CHL cells

Test Substance

Description of the test substance: Neopentyl glycol
Purity Grade: 99.1%
Vehicle - Solvent: Distilled water

Test Method and Conditions


Exposure

Exposure: 0-1.00 mg/ml
Exposure comments: The exposure doses are: 0, 0.25, 0.50, 1.00mg/ml.

Test Results

<table>
<thead>
<tr>
<th>Organ</th>
<th>Effect</th>
<th>Rev.</th>
<th>OnSet</th>
<th>Sex</th>
<th>Affected in Exposed - Controls</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>NEF</td>
</tr>
</tbody>
</table>

The test material was classified as "negative" under the experimental condition used.

References

Primary Reference: #URMMT*

Secondary Reference: !SIDSP*
Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)
Study

End Point : REPRODUCTION
Chemical Name : 1,3-Propanediol, 2,2-dimethyl-
CAS Number : 126-30-7
Study type : LAB

Test Subject

Organism | Medium | Specification | Route | Lifestage | Sex | Number exposed | Number controls
--- | --- | --- | --- | --- | --- | --- | ---
RAT ORL | | | | | | | |
Species/strain/system : Slc: SD strain

Test Substance

Description of the test substance : Neopentyl glycol
Purity Grade : 99.1%
Vehicle - Solvent : Distilled water

Test Method and Conditions

Test method description : OECD Combined Repeated Dose and Reproductive/Developmental Toxicity Screening Test. Killing day: male: day 43; female: day 4 of lactation. GLP: yes.

Exposure

Exposure comments : The exposure doses are: 0(vehicle), 100, 300, 1000mg/kg/day. Administration period: male: 42 days; female: from 14 day before mating to day 3 of lactation.

Test Results

<table>
<thead>
<tr>
<th>Organ</th>
<th>Effect</th>
<th>Rev.</th>
<th>OnSet</th>
<th>Sex</th>
<th>Exposed - Controls</th>
</tr>
</thead>
<tbody>
<tr>
<td>REPRO</td>
<td>NEF</td>
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<td></td>
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</tr>
<tr>
<td>OFSPR</td>
<td>NEF</td>
<td></td>
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<td></td>
<td></td>
</tr>
</tbody>
</table>

There were no effect of test substance on copulation, fertility and estrus cycle of rats. Delivery was normal for dams except for one animal of control group. No effects of test substance on dams during the lactation period were observed.

NOAEL

For P generation: 1000mg/kg

NOAEL

For F1 generation: 1000mg/kg

General Comments : Estimated Doses of Low Concern: EDLC = NOAEL/UF = 1000/100 = 10.0mg/kg/day.
References

Primary Reference:
#URMHW*

Secondary Reference:
!SIDSP*
Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)
Study

End Point : TERATOGENICITY
Chemical Name : Neopentyl glycol
CAS Number : 126-30-7
Study type : LAB

Test Subject

<table>
<thead>
<tr>
<th>Organism</th>
<th>Medium</th>
<th>Specification</th>
<th>Route</th>
<th>Lifestage</th>
<th>Sex</th>
<th>Number exposed</th>
<th>Number controls</th>
</tr>
</thead>
<tbody>
<tr>
<td>RAT</td>
<td>ORL</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Species/strain/system : Slc: SD strain

Test Method and Conditions

Test method description : OECD Reproduction/Developmental Toxicity Screening Test

Exposure

Dose / Concentration : 100-1000 mg/kg BW
Exposure comments : In utero exposure to the maternal doses of 0, 100, 300, 1000mg/kg body weight/day of neopentyl glycol for assessment of teratogenic potential.

Test Results

<table>
<thead>
<tr>
<th>Organ</th>
<th>Effect</th>
<th>Rev.</th>
<th>OnSet</th>
<th>Sex</th>
<th>Exposed - Controls</th>
</tr>
</thead>
<tbody>
<tr>
<td>FETUS</td>
<td>NEF</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Stillborn, dead pups and pups sacrificed at day 4 of lactation showed no abnormal gross findings suggesting any influence on fetal development from the test substance.

General Comments : External examination of pups revealed no increase in appearance of abnormal pups to be caused by the test substance. Body weight gain of pups was normal up to day 4 of lactation. In the final comment the author stated that no effect on developmental toxicity was observed.

References

Primary Reference : #URMHW*
Unpublished Report on Combined Repeated Dose and Reproductive/Developmental Toxicity Screening Test conducted by the Ministry of Health and Welfare (MHW), Japan

Secondary Reference : !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, 14-15, (1993)
Study

End Point: AQUATIC ACUTE TOXICITY
Chemical Name: 1,3-Propanediol, 2,2-dimethyl
CAS Number: 126-30-7

Species/strain/system: Orange-red Killifish (Oryzias latipes)
Exposure Period: 24-96 h
Exposure comments: The same doses were also tested for 48h and 72h.

Test Method and Conditions

Test method description: Semi-static

Test Results

<table>
<thead>
<tr>
<th>Organism</th>
<th>Medium</th>
<th>Spec.</th>
<th>Route</th>
<th>Lifestage</th>
<th>Sex</th>
<th>Effect</th>
<th>Effect Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>FISH</td>
<td>AQ</td>
<td>ESTUA</td>
<td></td>
<td></td>
<td></td>
<td>LC0</td>
<td>LC0 = 555mg/l (reported as 555ppm) for 24, 48, 72 and 96 hours, LC50 = &gt; 1000mg/l (reported as &gt; 1000ppm (w/v)).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>LC50</td>
<td></td>
</tr>
</tbody>
</table>

References

Primary Reference: #UREAF*
Unpublished Report on Toxicity to Fish Test conducted by Environmental Agency, Japan

Secondary Reference: !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

Study

End Point: AQUATIC ACUTE TOXICITY
Chemical Name: 1,3-Propanediol, 2,2-dimethyl
CAS Number: 126-30-7

Species/strain/system: Orange-red Killifish (Oryzias latipes)
Exposure Period: 48 h

Test Substance

Impurities: Water 0.03%, neopentyl hydroxy pivalate 0.44%, formic acid 0.002%

Test Method and Conditions

Test method description: JIS K0102. Static test.

Test Results

<table>
<thead>
<tr>
<th>Organism</th>
<th>Medium</th>
<th>Spec.</th>
<th>Route</th>
<th>Lifestage</th>
<th>Sex</th>
<th>Effect</th>
<th>Effect Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>FISH</td>
<td>ESTUA</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>LC50</td>
<td>&gt; 1000mg/l (reported &gt; 1000 ppm)</td>
</tr>
</tbody>
</table>

IRPTC Data Profile
References

Primary Reference : #UREAF*
Unpublished Report on Toxicity to Fish Test conducted by Environmental Agency, Japan

Secondary Reference : !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)
Aquatic Toxicity

Study

End Point : AQUATIC TOXICITY
Chemical Name : 1,3-Propanediol, 2,2-dimethyl-
CAS Number : 126-30-7

Test Subject

Organism | Medium | Specification | Route | Lifestage | Sex | Number exposed | Number controls
---------|--------|---------------|-------|-----------|-----|----------------|------------------
ALGAE

Species/strain/system : Algae (Selenastrum capricornutum)

Test Substance

Description of the test substance : Neopentyl glycol
Purity Grade : >99%

Test Method and Conditions

Test method description : OECD Test Guideline. GLP: no

Exposure

Exposure Period : 72 h
Dose / Concentration : >1000 mg/l w/v

Test Results

<table>
<thead>
<tr>
<th>Organ</th>
<th>Effect</th>
<th>Rev.</th>
<th>OnSet</th>
<th>Sex</th>
<th>Exposed</th>
<th>Controls</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Affected in</td>
<td></td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>EBC50</td>
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<td></td>
</tr>
</tbody>
</table>

Effective concentration (reported as EBC50 > 1000ppm (w/v) for 42h)

References

Primary Reference : #UREAA*

Secondary Reference : !SIDSP*
Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)
**Study**

*End Point*: AQUATIC TOXICITY  
*Chemical Name*: 1,3-Propanediol, 2,2-dimethyl  
*CAS Number*: 126-30-7

**Test Subject**

<table>
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<tr>
<th>Organism</th>
<th>Medium</th>
<th>Specification</th>
<th>Route</th>
<th>Lifestage</th>
<th>Sex</th>
<th>Number exposed</th>
<th>Number controls</th>
</tr>
</thead>
<tbody>
<tr>
<td>CRUS</td>
<td>AQ</td>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
</tbody>
</table>

*Species/strain/system*: Water flea (Daphnia magna)

**Test Substance**

*Purity Grade*: 98%

**Test Method and Conditions**

*Test method description*: Static test. Method used to calculate EC values: Probit method.

**Exposure**

*Exposure Period*: 21 d  
24–48 h

**Test Results**

<table>
<thead>
<tr>
<th>Organ</th>
<th>Effect</th>
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<th>Sex</th>
<th>Exposed - Controls</th>
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</table>

*NOEC*: Maximum concentration at which no effect was observed > 1000ppm (w/v) for 21 days.

*EC0*: For 24h lowest dose without effect: > 1000ppm (w/v)

*EC50*: For 24h lowest dose without effect: > 1000ppm (w/v)

**References**

*Primary Reference*: #URTEA*  
Unpublished Toxicity Test conducted by the Environmental Agency, (EA), Japan

*Secondary Reference*: !SIDSP*  
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)
Aquatic Toxicity

**Study**

*End Point:* AQUATIC TOXICITY

*Chemical Name:* 1,3-Propanediol, 2,2-dimethyl-

*CAS Number:* 126-30-7

**Test Subject**

<table>
<thead>
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<th>Organism</th>
<th>Medium</th>
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<th>Route</th>
<th>Lifestage</th>
<th>Sex</th>
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<th>Number controls</th>
</tr>
</thead>
<tbody>
<tr>
<td>CRUS</td>
<td></td>
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</tr>
</tbody>
</table>

*Species/strain/system:* Water flea (Daphnia magna)

**Test Substance**

*Description of the test substance:* Neopentyl glycol

*Purity Grade:* >98%

**Test Method and Conditions**

*Test method description:* GLP: no. Probit method used to calculate these values.

**Exposure**

*Exposure Type:* ACUTE

*Exposure Period:* 24-48 h

*Dose / Concentration:* >1000 ppm w/v

**Test Results**

<table>
<thead>
<tr>
<th>Organ</th>
<th>Effect</th>
<th>Rev.</th>
<th>OnSet</th>
<th>Sex</th>
<th>Affected in Exposed - Controls</th>
</tr>
</thead>
<tbody>
<tr>
<td>--------</td>
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<td>--------------------------------</td>
</tr>
</tbody>
</table>

**EC0**

The 24h EC0 and EC50 are higher than 1000ppm w/v.

**References**

*Primary Reference:* #URTEA*

Unpublished Toxicity Test conducted by the Environmental Agency, (EA), Japan, (1993)

*Secondary Reference:* !SIDSP*

Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)