FOREWORD

INTRODUCTION

DEHYDRO-BETA-LINALOOL

CAS N°: 29171-20-8
Identifiers, Physical and Chemical properties

Substance

**End Point**: IDENTIFIERS, PHYSICAL AND CHEMICAL PROPERTIES

**Chemical Name**: 6-Octen-1-yn-3-ol, 3,7-dimethyl-

**Common Name**: Dehydro-.beta.-linalool

**CAS Number**: 29171-20-8

Synonyms

Dehydrolinalool
Linalool, dehydro-

Properties & Definitions

- **Molecular Formula**: C10H16O
- **Molecular Weight**: 152.24
- **Melting Point**: -57°C
- **Boiling Point**: 198°C
- **Flash Point**: 85°C (c-cup)
- **Density**: 0.88 g/mL at 20°C
- **Vapour Pressure**: 1.112E-2 kPa(8.34 mmHg) at 20°C
- **Octanol/Water Partition Coefficient**: log Pow = 2.61 at 25°C
- **Water Solubility**: 2.45 g/L at 20°C
- **Impurities**: Acetic acid isopropyl ester maximum 0.5%; 1-methyl-2-methylene-3-isopropenylcyclopentanol (2 isomers) each maximum 0.2%; methylheptenone (.alpha. and .beta.) maximum 0.5%.

**General Comments**: Ignition temperature 270°C. pH in water: neutral. Exposure to air may cause yellowing and deterioration. Moderately volatile. To measure water solubility flask method is used.

Overall Evaluation

PRESENTLY OF LOW PRIORITY FOR FURTHER WORK

Dehydrolinalool is acute barely toxic but irritant to skin and eyes. It is of low subacute toxicity in rats (NOAEL males: 200 mg/kg; NOAEL females: 600 mg/kg). No signs of a teratogenic action were observed in a preliminary reproductive toxicity screening test. In the Ames test and in a chromosome aberration test in the presence of a metabolising system DLL did not induce genotoxic activity. Without metabolic activation DLL showed marginal clastogenic activity in vitro. In the mouse micronucleus test, DLL was non-clastogenic up to the limit dose of 2000 mg/kg.

Dehydrolinalool is moderately toxic to water organisms. It is readily biodegradable and no bioaccumulation is expected.

DLL is exclusively used as an intermediate for further chemical conversion. Manufacturing and processing is the only relevant source for releases into the environment. General environmental exposure can be excluded. The potential environmental concentration is expected to be highest near the production site, but PEC estimations gave no reason for concern even under worst case assumptions.

Under the known conditions of use dehydrolinalool is very unlikely to present a risk to human health. The general population is not exposed. At the workplace the chemical is produced and handled as a hazardous material, though toxic effects seem to be very unlikely based on the available test results.

ENVIRONMENTAL EXPOSURE

**SOURCES, PARTITIONING AND FATE**

Dehydrolinalool is a water soluble, moderately volatile, readily biodegradable chemical without potential to bioaccumulate. It is exclusively used as an intermediate for further chemical conversion. Finland and Germany positively confirmed that no end uses are known in their countries. Production, therefore, is the only relevant...
source for releases into the environment. Based on its properties and on its use pattern, potential environmental concentrations are expected to be highest near the production site. Further exposure assessments using global models as proposed by the provisional OECD-guidance will in our view not lead to improved knowledge in the present case.

EMISSION TO WASTE WATER

In Germany, emission to water during production and processing has been reported to be negligible. In Switzerland, the manufacturing procedure of DLL is a continuous process carried out in a closed system. All reagents and solvents used for the synthesis of DLL are conveyed to the reaction vessel through closed pipelines from storage tanks and storage vessels.

After the reaction is completed, the crude DLL is pumped from the reaction vessel through a closed tube to an extractor where the reaction mixture is washed with hot water and cleared of water-soluble byproducts. The washing water of this last production step contains both water-soluble inorganic impurities (such as salts) and small amounts of DLL. It is discharged through the drain valve of the extractor to the sewage system which is connected to the Visp regional waste water treatment plant.

The amount of DLL released continuously with the waste water is in the order of 50 kg per day.

The predicted environmental concentration (PEC) of DLL in the river Rhone, the receiving water of the Visp regional waste water treatment plant, can be calculated using the method for the "calculation of substance concentrations in waste water, receiving water and sewage sludge" published in the document "Guide to Self Supervision" by the Swiss Federal Office of Environment, Forests and Landscape and using the values for W and b for the worst case as follows:

\[
\text{PEC} = \frac{\text{ASD} \times f}{W} \times b = \frac{50 \times 10^6 \times 0.04}{15 \times 10^6} \times 32 = 0.004 \text{ mg/L}
\]

\[
\text{PEC} = \text{Concentration in the receiving water}
\]

\[
\text{ASD} = \text{Amount of substance discharged into waste water} : 50 \text{ kg/day}
\]

\[
\text{f} = \text{Percentage which cannot be eliminated} : 0.04
\]

(DLL is biodegradable: 96% DOC elimination in 28 days; OECD 302 B: Inherent biodegradability (Zahn-Wellens test))

\[
W = \text{Daily amount of waste water in the regional waste water treatment plant: } 15 \times 10^6 \text{ L/day (the amount differs from } 15000 \text{ mE+3/day to } 18000 \text{ mE+3/day)}
\]

\[
b = \text{Dilution factor in the river Rhone : } 32 \text{ under worst case conditions (water passage of the Rhone differs from } 20000 \text{ mE+3/hour (winter) to } 600000 \text{ mE+3/hour (summer))}
\]

\[
20000 \text{ mE+3/hour } \times 24/15000 \text{ mE+3/day} = 32
\]

The result of the inherent biodegradability test shows that the biodegradation of DLL under the test conditions is relatively slow, but it also shows that the compound is degraded almost completely after adaptation of the microorganisms. This adaptation will also take place in the waste water treatment plant, since the waste water containing DLL is continuously discharged in the sewage.

Taking these facts into account the value for the factor f (0.04) might nevertheless be somewhat too optimistic. Thus, based on the value for the amount degraded after 14 days (53%) in the inherent biodegradability test and based on the result of the ready biodegradability test (55% biological oxygen demand in 28 days), the calculation is as follows:

\[
\text{PEC} = 50 \times 10^6 \times 0.5/15 \times 10^6 \times 32 = 0.05 \text{ mg/L}
\]

This result - 0.05 mg/L - is the theoretical concentration of DLL calculated under worst-case conditions. Actual figures resulting from measurements of the DLL concentration in the outlet of the waste water treatment plant are not available.

EMISSION TO AIR

SWITZERLAND:
The only possible source of emission to the air consists in the filling process of barrels. Since the total quantity transferred to barrels is relatively small (<10 tonnes/year) and on the basis of the relatively low vapour pressure (1.112E-2 kPa) as well as the high boiling point (198°C) the amount of DLL emitted to the air is negligible. Actual figures resulting from measurements are not available.
GERMANY:
Emissions into the air during production and processing were reported to be about 5 kg/year.

CONSUMER EXPOSURE

Dehydrolinalool produced by the Swiss manufacturer is not used as an end product in any consumer product or any application form. To our knowledge neither is any DLL produced by other manufacturers processed in consumer products. Indirect consumer exposure is also not expected to occur, because DLL is released only in small quantities into the environment and it is rapidly degraded.

OCCUPATIONAL EXPOSURE

The entire DLL manufacturing process and its following transformations to other chemical substances are carried out in closed systems as are the transfusion operations for the small part required for transportation. The only open-handled operation is the process of filling the 200 L barrels. As DLL has a low vapour pressure and a high boiling point, there will be no consequences for exposure at the place work. Possible exposure is prevented by adequate air vent devices.

ENVIRONMENT

Dehydrolinalool is considered to be moderately toxic to fish, daphnids and algae. It shows a good water solubility and is readily biodegradable. As the log Pow is 2.61 no bioaccumulation potential is expected.

The hazard assessment for the aquatic organisms is based on the procedure described in the OECD “Guidance for assessment of aquatic effects”.

For the calculation of the maximum tolerable concentration (MTC) the NOAEL of the rainbow trout was selected:

- LC50, Rainbow trout > 18 mg/L (NOAEL) > 40 mg/L
- EC50, Daphnids: 45 mg/L
- EC50, Algae: 48 mg/L

An assessment factor of 100 is used as acute toxicity studies for algae, crustaceans and fish are available.

MTC = 18/100 = 0.18 mg/L

The predicted environmental concentration (PEC) for the worst case was calculated to be 0.05 mg/L.

A comparison of MTC with PEC gives a value of

MTC/PEC = 0.18 mg/L/0.05 mg/L = 3.6

CONCLUSION

Locally DLL is of low concern to the aquatic environment, unless the conditions near the production site are less favourable than at the plant in Switzerland. Globally DLL is of no environmental concern. There are no diffuse releases into the environment, the substance is readily biodegradable and shows no tendency for bioaccumulation.

INITIAL ASSESSMENT

Dehydrolinalool is an intermediate used exclusively for subsequent chemical syntheses. It is not used as an end product in consumer products or in any application form. DLL is manufactured and processed in closed systems, i.e. the product itself and all reagents and solvents for its syntheses are handled in closed tubes and vessels. Most of the DLL manufactured is used at the place of production. Only a small part of the production is sent off-site to a company belonging to the Roche group for further chemical processing. Thus DLL is classified as an "isolated intermediate with controlled transport" according to OECD.

HUMAN HEALTH

Dehydrolinalool is considered to be acute barely toxic, but irritating to skin and eyes.

In a 28-day oral study, DLL was shown to be of low subacute toxicity in rats with regard to hematological and clinical chemistry parameters. The compound induced treatment-related hypersalivation and to some extent sedation in the high-dose group. In males, DLL induced hyaline droplets nephropathy, essentially at high dose
levels. This nephropathy is known to be specific in male rats, whereas hyaline droplet inducers do not predispose humans to develop nephropathy. At the concentration of 200 mg/kg/day the only observed effect was a pre-stage of hyaline droplets nephropathy, which was also seen in some control animals.

The No observed adverse effects levels (NOAEL) in a preliminary reproductive toxicity screening test were 750 mg/kg for the males, 200 mg/kg for the offspring and 50 mg/kg for the dams. Thus 50 mg/kg was defined as non-toxic dose (NTD).

From this data an estimated dose of low concern (EDLC) can be calculated, taking into account an uncertainty factor UF of 100:

\[
\text{EDLC} = \frac{\text{NTD}}{\text{UF}} = \frac{50}{100} = 0.5 \text{ mg/kg/day}
\]

No consumer exposure is given for DLL since the substance is used as an end product in any consumer product or any application form. Under normal conditions and the usual safety precautions, an occupational exposure is not to be expected either.

Considering this low expected human exposure it can be assumed that also the estimated human exposure (EHE) is low. Therefore the substance is estimated to be of low concern for the reproduction and developmental toxicity.

DLL did not induce mutagenic activity in the Ames test nor did it induce clastogenic activity in the presence of mammalian metabolising system in the chromosome aberration test (CHO cells). However, DLL per se (without metabolic activation) was clastogenic at dose levels that were also cytotoxic. In a non bacterial in vivo test (micronucleus assay in mouse bone marrow) DLL was non-clastogenic. The results demonstrate, that is is very likely that DLL is detoxified under in vivo conditions. Therefore its potential risk for humans is low.

Conclusion:
Based on the EDLC/EHE ratio DLL is considered to be of low concern to human health.

CONCLUSIONS AND RECOMMENDATIONS

Based on the available information it can be concluded that dehydrolinalool does not present a hazard to human health or the environment and may be classified as chemical of low concern.

No further tests are required.
Waste water sampling is recommended for producers, if the local conditions are less favourable than at the Swiss plant (e.g. lower dilution factor).
## Production-Trade

**Chemical Name**: 6-Octen-1-yn-3-ol, 3,7-dimethyl-<br>**CAS Number**: 29171-20-8<br>**Geographic Area**: CHE

### Production

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Year</th>
<th>General Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>10000-15000 t - P</td>
<td>1989</td>
<td>Dehydrolinalool is manufactured at one production site in Switzerland (Teranol, Lalden).</td>
</tr>
</tbody>
</table>

### References


## Production-Trade

**Chemical Name**: 6-Octen-1-yn-3-ol, 3,7-dimethyl-<br>**CAS Number**: 29171-20-8<br>**Geographic Area**: DEU

### Production

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Year</th>
<th>General Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>&gt;1000 t - P</td>
<td>1992</td>
<td>According to OECD/SIDS knowledge, there is one production site in Germany.</td>
</tr>
</tbody>
</table>

### References

*!SIDSP*<br>OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

## Production-Trade

**Chemical Name**: 6-Octen-1-yn-3-ol, 3,7-dimethyl-<br>**CAS Number**: 29171-20-8<br>**Geographic Area**: WORLD

### Production

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Year</th>
</tr>
</thead>
<tbody>
<tr>
<td>10000-15000 t - P</td>
<td>1991</td>
</tr>
<tr>
<td>11000 t - P</td>
<td></td>
</tr>
</tbody>
</table>
References

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)
Uses

Chemical Name: 6-Octen-1-yn-3-ol, 3,7-dimethyl-
CAS Number: 29171-20-8

Use

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Year</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>DLL is an intermediate for further chemical synthesis. The whole production is used for synthesis of fragrances and for other intermediates in the manufacture of pharmaceutical substances and vitamins. Thus DLL does not appear in any consumer product. The greatest part of the manufactured DLL is consumed at the place of production.</td>
</tr>
</tbody>
</table>

References

Secondary References: !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)
Study

End Point : Pathway into the Environment and Environmental Fate.
Chemical Name : 6-Octen-1-yn-3-ol, 3,7-dimethyl-
CAS Number : 29171-20-8
Geographic Area : CHE

Pathway and Transport

Pathway : AIR AQ
Pathway description : Emission to air in the filling process of barrels.

Quantity Transported

<table>
<thead>
<tr>
<th>Medium</th>
<th>to Medium</th>
<th>Quantity</th>
<th>Time</th>
<th>Year</th>
<th>to Year</th>
</tr>
</thead>
<tbody>
<tr>
<td>AIR</td>
<td>AQ WASTE</td>
<td>50 kg</td>
<td>d</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The washing water from the last production step of DLL contains both water-soluble inorganic impurities (such as salts) and small amounts of DLL. It is discharged to the sewage system connected to the regional waste water treatment plant (Visp).

References

Secondary Reference : !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point : Pathway into the Environment and Environmental Fate.
Chemical Name : 6-Octen-1-yn-3-ol, 3,7-dimethyl-
CAS Number : 29171-20-8
Geographic Area : DEU

Pathway and Transport

Pathway : AQ AIR
Pathway description : Emission during production and processing.

Quantity Transported

<table>
<thead>
<tr>
<th>Medium</th>
<th>to Medium</th>
<th>Quantity</th>
<th>Time</th>
<th>Year</th>
<th>to Year</th>
</tr>
</thead>
<tbody>
<tr>
<td>AIR</td>
<td>5 kg</td>
<td>y</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Emission to water during production and processing has been reported to be negligible.

General Comments : The manufacturing procedures applied and the safety precaution measures exclude further direct environmental exposure of DLL under normal conditions during production, transport and subsequent processing.
References

Secondary Reference: !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)
Study

End Point : CONCENTRATION
Chemical Name : 6-Octen-1-yn-3-ol, 3,7-dimethyl-
CAS Number : 29171-20-8
Study type : FIELD
Geographic Area : CHE
Area Specifications : E

Test Subject

Organism Medium Specification Lifestage Sex
AQ FRESH

Species/strain/system : The Rhone river receiving water of the regional waste water treatment plant (Visp).

Test Method and Conditions

Test method description : Calculation of substance concentrations in waste water, receiving water and sewage sludge. (Published in the document "Guide to Self Supervision" by the Swiss Federal Office of Environment, Forests and Landscape.

Test Results

Matrix Concentrations Spec. Date

0.05 mg/L
PEC: predicted environmental concentrations in the river Rhone. This result is the theoretical concentration of DLL calculated under worst-case conditions assuming that the percentage which cannot be eliminated is 0.5.

0.004 mg/L
PEC in the river Rhone, assuming that the percentage which cannot be eliminated is 0.04 which is considered somewhat optimistic.

References

Secondary Reference : !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)
Study

End Point : BIODEGRADATION
Chemical Name : 6-Octen-1-yn-3-ol, 3,7-dimethyl-
CAS Number : 29171-20-8
Study type : LAB

Test Subject

Organism Medium Specification
MCR AQ SLUDG
Species/strain/system : Sewage treatment 50% from communal WWTP, 50% from industrial
WWTP (Waste Water Treatment Plant).

Test Substance

Purity Grade : 98%

Test Method and Conditions

Test method description : Zahn-Wellens Test. (Inherent biodegradability according to OECD
302B). GLP: no
(An)aerobic : AEROB

Exposure

Exposure Period : 5-28 d
Dose / Concentration : 300 mg/L
Exposure comments : Concentrations were also measured after 7 and 14 days.

Test Results

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Time</th>
<th>Comments on result</th>
</tr>
</thead>
<tbody>
<tr>
<td>18 %</td>
<td>AV 5 d</td>
<td>DOC elimination</td>
</tr>
<tr>
<td>35 %</td>
<td>AV 7 d</td>
<td>DOC elimination</td>
</tr>
<tr>
<td>53 %</td>
<td>AV 14 d</td>
<td>DOC elimination</td>
</tr>
<tr>
<td>96 %</td>
<td>AV 28 d</td>
<td>DOC elimination</td>
</tr>
</tbody>
</table>

Nominal concentration of 300 mg/L corresponding to 240 mg DOC/L
(measured for control).

References

Primary Reference : #URHLR*
Hoffmann-La Roche. Unpublished Report Hoffmann-la-Roche, E-5/85,
(1990)

Secondary Reference : !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High
Production Volume Chemicals Programme, (1994)
**Study**

<table>
<thead>
<tr>
<th>End Point</th>
<th>BIODEGRADATION</th>
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</thead>
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<tr>
<td>Chemical Name</td>
<td>6-Octen-1-yn-3-ol, 3,7-dimethyl-</td>
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<tr>
<td>CAS Number</td>
<td>29171-20-8</td>
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<tr>
<td>Study type</td>
<td>LAB</td>
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**Test Subject**

<table>
<thead>
<tr>
<th>Organism</th>
<th>Medium</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>MCR</td>
<td>AQ</td>
<td>SLUDG</td>
</tr>
</tbody>
</table>

| Species/strain/system     | Sewage treatment 50% from communal WWTP, 50% from industrial WWTP (Waste Water Treatment Plant). |

**Test Substance**

| Purity Grade | 98% |

**Test Method and Conditions**

| Test method description | OECD Guideline 301D. Closed Bottle Test; GLP: no |

| (An)aerobic | AEROB |

**Test Results**

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Time</th>
<th>Comments on result</th>
</tr>
</thead>
<tbody>
<tr>
<td>55 %</td>
<td>AV</td>
<td>28 d</td>
</tr>
</tbody>
</table>

**References**

- **Primary Reference**: #URHLR*

- **Secondary Reference**: !SIDSP*
  OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)
Study

<table>
<thead>
<tr>
<th>End Point</th>
<th>BIODEGRADATION</th>
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<tr>
<td>Chemical Name</td>
<td>6-Octen-1-yn-3-ol, 3,7-dimethyl-</td>
</tr>
<tr>
<td>CAS Number</td>
<td>29171-20-8</td>
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<tr>
<td>Study type</td>
<td>LAB</td>
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</table>

Test Subject

<table>
<thead>
<tr>
<th>Organism</th>
<th>Medium</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>MCR</td>
<td>AQ</td>
<td>SLUDG</td>
</tr>
</tbody>
</table>

Species/strain/system : Sewage treatment. 50% from Communal WWTP, 50% from industrial WWTP (Waste Water Treatment Plant).

Test Substance

| Purity Grade | 99% |

Test Method and Conditions

<table>
<thead>
<tr>
<th>Test method description</th>
<th>OECD Guideline 301E. Modified Screening Test. GLP: no</th>
</tr>
</thead>
<tbody>
<tr>
<td>(An)aerobic</td>
<td>AEROB</td>
</tr>
</tbody>
</table>

Test Results

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Time</th>
<th>Comments on result</th>
</tr>
</thead>
<tbody>
<tr>
<td>&gt;70 %</td>
<td>AV</td>
<td>28 d</td>
</tr>
</tbody>
</table>

General Comments : Based on these results DLL can be considered as "readily biodegradable".

References

Primary Reference : #URBSF*  
BASF. BASF, Unpublished Report, (1990)

Secondary Reference : !SIDSP*  
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)
Bioconcentration

Study

End Point : BIOCONCENTRATION
Chemical Name : 6-Octen-1-yn-3-ol, 3,7-dimethyl-
CAS Number : 29171-20-8

Test Results

General Comments : Chemical does not have potential to bioaccumulate.

References

Secondary Reference : !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)
Mammalian Acute Toxicity

Study

End Point: MAMMALIAN ACUTE TOXICITY
Chemical Name: 6-Octen-1-yn-3-ol, 3,7-dimethyl-
CAS Number: 29171-20-8
Study type: LAB

Species/strain/system: No information on strain provided
Exposure Type: SHORT

Test Substance

Purity Grade: 98%

Test Method and Conditions

Test method description: Internal method, Hoffmann-La Roche, Basel (repeated dose toxicity). GLP: no

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>MOUSE</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>LD50</td>
<td>LD50 was established as 1060 mg/kg (10 days following 5th administration).</td>
</tr>
</tbody>
</table>

References

Primary Reference: #URHLR*
Hoffmann-La Roche. Unpublished Report Hoffmann-la-Roche, RCB-156 425

Secondary Reference: !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point: MAMMALIAN ACUTE TOXICITY
Chemical Name: 6-Octen-1-yn-3-ol, 3,7-dimethyl-
CAS Number: 29171-20-8

Test Method and Conditions

Test method description: BASF internal method. GLP: no

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 LD50 for the rat was calculated as 3100 mg/kg.</td>
</tr>
</tbody>
</table>
References

Primary Reference: #URBSF*
BASF. BASF, Unpublished Report, 77/277

Secondary Reference: !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point: MAMMALIAN ACUTE TOXICITY
Chemical Name: 6-Octen-1-yn-3-ol, 3,7-dimethyl-
CAS Number: 29171-20-8

Species/strain/system: No information on the strain provided
Exposure Period: 7 h
Exposure comments: Saturated atmosphere at 20°C for 7 hours.

Test Substance

Vehicle - Solvent: air

Test Method and Conditions

Test method description: Under the influence of OECD Guideline No. 403. GLP: no

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>IHL</td>
<td>ADULT</td>
<td></td>
<td>LD50</td>
<td></td>
<td></td>
<td>Inhalation LD50 for the rat could not be calculated. There was no mortality after 7 hours exposure to saturated concentration of the test substance in the air.</td>
</tr>
</tbody>
</table>

References

Primary Reference: #URBSF*
BASF. BASF, Unpublished Report

Secondary Reference: !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point: MAMMALIAN ACUTE TOXICITY
Chemical Name: 6-Octen-1-yn-3-ol, 3,7-dimethyl-
CAS Number: 29171-20-8

Exposure comments: 10 day single administration study.
Test Method and Conditions

Test method description: Hoffmann-La Roche internal method. GLP: no

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>MOUSE</td>
<td>ORL</td>
<td>ADULT</td>
<td></td>
<td></td>
<td></td>
<td>LD50</td>
<td>Oral LD50 for the mouse was calculated as 4240 mg/kg.</td>
</tr>
</tbody>
</table>

References

Primary Reference: #URHLR*
Hoffmann-La Roche. Unpublished Report Hoffmann-la-Roche, RCB-156 425

Secondary Reference: !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)
Study

End Point: MAMMALIAN TOXICITY
Chemical Name: 6-Octen-1-yn-3-ol, 3,7-dimethyl-
CAS Number: 29171-20-8
Study type: LAB

Test Subject

Organism | Medium | Specification | Route | Lifestage | Sex | Number exposed | Number controls
---|---|---|---|---|---|---|---
RAT | ORL | ADULT | M | 10-14 | F | 10-14 |

Species/strain/system: Hanlbm:Wist(SPF) rats

Test Substance

Purity Grade: 99.5%

Test Method and Conditions

Test method description: Internal method, Hoffmann-La Roche. GLP: yes

Exposure

Exposure Type: SHORT
Exposure Period: 28 d
Dose / Concentration: 200-1000 mg/kg
Exposure comments: Groups of 10 or 14 male and 10 or 14 female rats were treated orally (by gavage) with 0 mg/kg/day, 200 mg/kg/day, 600 mg/kg/day (400 mg/kg/day for one week) and 1000 mg/kg/day (900 mg/kg/day for 2 days) of the intermediate dehydrolinalool for a 4-week period.

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>CNS</td>
<td>DECR</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Sedative effect was observed in the high-dose group.

LIVER SIZE
A slight increase in relative adjusted liver weight occurred.

KIDNY STRUC M
A dose related increase in the incidence and severity of hyaline droplet nephropathy was observed in the males of the mid and high-dose groups.

GIT EXOC
Compound induced hypersalivation was observed in all groups.

DEATH F 2
Two females showing increased salivation and sedation in high-dose group. Though a treatment-related effect cannot be excluded, this is considered to be of minor toxicological relevance.

General Comments: Hyaline droplets nephropathy is male rat-specific and was never found in common mammalian species nor in humans.
References

Primary Reference: #URHLR*

Secondary Reference: !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)
Study

- **End Point**: MUTAGENICITY
- **Chemical Name**: 6-Octen-1-yn-3-ol, 3,7-dimethyl-
- **CAS Number**: 29171-20-8
- **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>BACT</td>
<td>VTR</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- **Species/strain/system**: Salmonella typhimurium

Test Substance

- **Purity Grade**: >99%

Test Method and Conditions

- **Test method description**: OECD Guideline 471 (+/- S9 Mix), Ames test. GLP: no

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>MUT</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The compound was negative for mutagenic effects in the tests with and without metabolic activation by S-9.

References

- **Primary Reference**: #URBSF*. BASF. BASF, Unpublished Report, 87/804
- **Secondary Reference**: !SIDSP*. OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

- **End Point**: MUTAGENICITY
- **Chemical Name**: Dehydro-.beta.-linalool
- **CAS Number**: 29171-20-8
- **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>BACT</td>
<td>VTR</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- **Species/strain/system**: Salmonella Typhimurium TA100, TA98
Mutagenicity

Test Substance

Purity Grade : >99%

Test Method and Conditions

Test method description : In accordance with OECD 471; reverse mutation assay (modified Ames test), liquid suspension assay. Both in the presence and in the absence of a metabolizing system from rat liver (S-9 mix).

Exposure

Dose / Concentration : 4-5000 ug/ PLATE
Exposure comments : The test was performed with following doses: 0, 4, 20, 100, 500, 1000, 2500 and 5000 ug/plate.

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>NEF</td>
<td>NEF</td>
<td>NEF</td>
<td>NEF</td>
<td>NEF</td>
<td>NEF</td>
</tr>
</tbody>
</table>

No increase in the number of His+ revertants was observed with and without metabolic activation.

CELL

A bacteriotoxic effect (reduced His- background growth, decrease in the number of His+ revertants) was observed depending on the test conditions from 1000 - 2500 ug/plate onward.

General Comments : Project No. of the study: 41M0638/904512

References

Primary Reference : #URBSF*

Secondary Reference : !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point : MUTAGENICITY
Chemical Name : 6-Octen-1-yn-3-ol, 3,7-dimethyl-
CAS Number : 29171-20-8
Study type : LAB

Test Subject

Organism Medium Specification Route Lifestage Sex Number exposed Number controls

HAMST VTR

Species/strain/system : CHO cells

Test Method and Conditions

Test method description : OECD Guideline No. 473, chromosomal aberration test; GLP: yes
Mutagenicity

Exposure

- **Exposure Type**: SHORT
- **Exposure Period**: 3 h
- **Dose / Concentration**: 100-300 µg/mL
- **Exposure comments**: Short time exposure without metabolic activation by S-9. The positive controls were treated with bleomycin or cyclophosphamide.

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>MUT</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

There was a clastogenic effect observed in the tests without metabolic activation.

References

- **Primary Reference**: #URHLR*
- **Secondary Reference**: !SIDSP*
  OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

- **End Point**: MUTAGENICITY
- **Chemical Name**: 6-Octen-1-yn-3-ol, 3,7-dimethyl-
- **CAS Number**: 29171-20-8
- **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>MOUSE</td>
<td>ORL</td>
<td>ADULT</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Test Method and Conditions

- **Test method description**: OECD Guideline No. 474 (micronucleus test). GLP: Yes

Exposure

- **Exposure Type**: SHORT
- **Dose / Concentration**: 500-2000 mg/kg
- **Exposure comments**: Micronucleus test was evaluated with oral gavage doses of 0, 500, 1000 and 2000 mg/kg body weight, with and without metabolic activation.

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>BONEM</td>
<td>CHNG</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

A slight antiproliferative effect was observed in the high dose groups at the 24 hour sampling time.

There was no chromosome breaking nor spindle disturbances demonstrated at any sampling time.
General Comments: According to the authors the micronucleus test confirmed the non-clastogenic effects of DLL in the presence of mammalian metabolizing system, thus indicating that there is no potential risk for humans.

References

Primary Reference: #URHLR*

Secondary Reference: !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)
Study

End Point : IRRITATION
Chemical Name : 6-Octen-1-yn-3-ol, 3,7-dimethyl-
CAS Number : 29171-20-8
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>RBT</td>
<td>OCU</td>
<td>ADULT</td>
<td></td>
<td>LAB</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Species/strain/system : No information on strain was provided

Test Substance

Purity Grade : >=99%

Test Method and Conditions

Test method description : BASF internal method, Draize-test (FDA). GLP: no

Exposure

Exposure Type : SHORT

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>--------------------------------</td>
</tr>
<tr>
<td>IRRIT</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

According to the test results as reported by the authors the compound is eye-irritating.

References

Primary Reference : #URBSF*
BASF. BASF, Unpublished Report, 77/277

Secondary Reference : !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)
Test Substance

Purity Grade : >=99%

Test Method and Conditions

Test method description : BASF internal method, Draize-test (FDA). GLP: no

Exposure

Exposure Type : SHORT

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>IRRIT</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

According to the test results as reported by the authors the compound is skin-irritating.

References

Primary Reference : #URBSF*
BASF. BASF, Unpublished Report, 77/277

Secondary Reference : !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)
**Study**

**End Point** : REPRODUCTION  
**Chemical Name** : 6-Octen-1-yn-3-ol, 3,7-dimethyl-  
**CAS Number** : 29171-20-8  
**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>20/GROUP</td>
<td>20</td>
<td>20</td>
<td>20</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>F</td>
<td>20/GROUP</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Species/strain/system** : FU-Albino rats

**Test Substance**

**Vehicle - Solvent** : Rape seed oil

**Test Method and Conditions**

**Test method description** : OECD Guideline for "Preliminary Reproduction Toxicity Screening Test". GLP: yes

**Exposure**

<table>
<thead>
<tr>
<th>Dose / Concentration</th>
<th>Exposure comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>50-750 mg/kg</td>
<td>Doses of: 0, 50, 200 or 750 mg/kg/day were administered by oral gavage from 14 days before mating, through mating and gestation period up to day 4 of lactation.</td>
</tr>
</tbody>
</table>

**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>BW</td>
<td>DECR</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Slight impairment of body weight gain was observed in males during the mating period and thereafter at 750 mg/kg/day dose group.

| CNS   | CHNG   |      |       |     |                                |
Transient ataxia and sedation was observed in females during the periods of gestation and lactation at 750 mg/kg/day dose.

| REPRO | CHNG   |      |       |     |                                |
Delivery complications were observed at 50 mg/kg/day (one out of 14) and at 750 mg/kg/day (3 out of 14 dams).

| ANS   | INCR   |      |       |     |                                |
Hypersalivation was observed in males and females at the dose level of 750 mg/kg/day.

**NOAEL**

No observed adverse effect level was at 750 mg/kg/day for the males.

**LOAEL**

The lowest observed adverse effect level was at 50 mg/kg/day for the dams.

**General Comments** : Delivery complications were categorised by the authors as possibly related to maternal toxicity. The affected dams either died or were sacrificed moribund during delivery. The duration of gestation, mean number of implants, resorption rate, mean number of pups per litter, mean pup weight and sex ratio were not significantly affected by the treatment in any dose group.
References

*Primary Reference*: #URHLR*

*Secondary Reference*: !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)
### Study

**End Point** : TERATOGENICITY  
**Chemical Name** : 6-Octen-1-yn-3-ol, 3,7-dimethyl-  
**CAS Number** : 29171-20-8  
**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>FETUS</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Species/strain/system** : FU-Albino rats

### Test Method and Conditions

**Test method description** : OECD Guideline for Preliminary Reproduction/Developmental Toxicity Screening Test. GLP: yes

### Exposure

**Exposure Type** : SHORT  
**Dose / Concentration** : 50-750 mg/kg  
**Exposure comments** : Doses of 0, 50, 200 or 750 mg/kg/day were administered to the parental animals, for evaluation of teratogenic effects.

### Test Results

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

At 750 mg/kg of maternal doses pup live birth and pup viability indices were slightly reduced.

**URS CHNG**

Increased incidence of abnormalities of the urinary system was noted at 750 mg/kg of maternal doses when compared to the control animals.

**NOAEL**

No observed adverse effect level for the offspring was at 200 mg/kg under the study conditions.

**General Comments** : No signs of teratogenic action were observed in any pup of dams which survived till the scheduled date of necropsy in any dose group.

### References

**Primary Reference** : #URHLR*  

**Secondary Reference** : !SIDSP*  
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)
Aquatic Acute Toxicity

Study

End Point : AQUATIC ACUTE TOXICITY
Chemical Name : 6-Octen-1-yn-3-ol, 3,7-dimethyl-
CAS Number : 29171-20-8

Species/strain/system : Golden orfe (Leuciscus idus)
Exposure Period : 96 h
Dose / Concentration : 21.5->46 mg/L

Test Substance

Purity Grade : 99%

Test Method and Conditions

Test method description : DIN 38412 T.15. Static test. GLP: no

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>FRESH</td>
<td></td>
<td></td>
<td></td>
<td>LC50</td>
<td>LC50 for 96 hours = 22-46 mg/L (nominal concentrations).</td>
</tr>
</tbody>
</table>

References

Primary Reference : #URBSF*

Secondary Reference : !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)
Aquatic Toxicity

Study

End Point : AQUATIC TOXICITY
Chemical Name : 6-Octen-1-yn-3-ol, 3,7-dimethyl-
CAS Number : 29171-20-8
Study type : LAB

Test Subject

Organism Medium Specification Route Lifestage Sex Number exposed Number controls

FISH AQ FRESH

Species/strain/system : Three-spined stickleback (Beta splendens)

Test Method and Conditions

Test method description : Test methods are not specified. GLP: no

Test Results

The aggressiveness is slightly inhibited.

References

Primary Reference : APFRAD
Binet, M. P. Annales Pharmaceutiques Francaises, 30(10), 653-658, (1972)

Secondary Reference : !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)
### Study

**End Point** : AQUATIC TOXICITY  
**Chemical Name** : 6-Octen-1-yn-3-ol, 3,7-dimethyl-  
**CAS Number** : 29171-20-8  
**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>ALGAE</td>
<td>AQ FRESH</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Species/strain/system** : Green algae (Scenedesmus subspicatus)

### Test Substance

**Purity Grade** : >=99%

### Test Method and Conditions

**Test method description** : DIN 38412 T.9; GLP: no

### Exposure

**Exposure Type** : ACUTE  
**Exposure Period** : 72-96 h  
**Dose / Concentration** : 34.6-100 mg/L

### 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>EC20</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

EC20 (effective concentration for toxicity) for 72 hours = 34.6 mg/L; EC20 for 96 hours = 38.5 mg/L.

**EC50**  
EC50 for 72 hours = 46 mg/L; EC50 for 96 hours = 47.9 mg/L.

**EC90**  
EC90 for 72 hours and 96 hours = 100 mg/L.

Th above results are nominal concentrations.

**General Comments** : SIDS does not provide specification of the toxic effect screened.

### References

**Primary Reference** : #URBSF*  

**Secondary Reference** : !SIDSP*  
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)
Study

End Point : AQUATIC TOXICITY
Chemical Name : 6-Octen-1-yn-3-ol, 3,7-dimethyl-
CAS Number : 29171-20-8
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>CRUS</td>
<td>AQ</td>
<td>FRESH</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Species/strain/system : Water flea (Daphnia magna, Strauss)

Test Substance

Purity Grade : 99%

Test Method and Conditions

Test method description : Directive 79/831/EWG, annex V C.2. GLP: no

Exposure

Exposure Type : ACUTE
Exposure Period : 24-48 h
Dose / Concentration : 25-100 mg/L
Exposure comments : Doses of 45.1 and 53.6 mg/L were also tested.

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></td>
</tr>
</tbody>
</table>

EC0
EC0 for 24 hours and 48 hours = 25 mg/L.

EC50
EC50 for 24 hours = 53.6 mg/L; EC50 for 48 hours = 45.1 mg/L.

EC100
EC100 for 24 hours and 48 hours = 100 mg/L.

The above results are nominal concentrations.

References

Primary Reference : #URBSF*

Secondary Reference : !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)
Study

End Point : AQUATIC TOXICITY
Chemical Name : 6-Octen-1-yn-3-ol, 3,7-dimethyl-
CAS Number : 29171-20-8

Test Subject

Organism Medium Specification Route Lifestage Sex Number exposed Number controls
FISH AQ FRESH

Species/strain/system : Rainbow trout (Oncorhynchus mykiss)

Test Method and Conditions

Test method description : OECD Guideline 203; static test; GLP: no

Exposure

Exposure Period : 48 h
Dose / Concentration : 40 mg/L

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>LC100</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

LC100 for 48 hours = 40 mg/L. (Nominal concentration).

References

Primary Reference : #URHLR*

Secondary Reference : !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point : AQUATIC TOXICITY
Chemical Name : 6-Octen-1-yn-3-ol, 3,7-dimethyl-
CAS Number : 29171-20-8
Study type : LAB

Test Subject

Organism Medium Specification Route Lifestage Sex Number exposed Number controls
FISH AQ FRESH

Species/strain/system : Rainbow trout (Oncorhynchus mykiss)
Aquatic Toxicity

Test Method and Conditions

Test method description : OECD Guideline 203; static test; GLP: no

Exposure

Exposure Type : ACUTE
Exposure Period : 48 h
Dose / Concentration : 18 mg/L

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>
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<td></td>
<td>NOEL</td>
</tr>
</tbody>
</table>

NOEL for 48 hours = 18 mg/L (nominal concentration).

References

Primary Reference : #URHLR*

Secondary Reference : !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point : AQUATIC TOXICITY
Chemical Name : 6-Octen-1-yn-3-ol, 3,7-dimethyl-
CAS Number : 29171-20-8
Study type : LAB

Test Subject

Organism Medium Specification Route Lifestage Sex Number exposed Number controls
FISH AQ FRESH

Species/strain/system : Golden orfe (Leuciscus idus)

Test Substance

Purity Grade : 99%

Test Method and Conditions

Test method description : DIN 38412 T.15; static test; GLP: no

Exposure

Exposure Period : 96 h
Dose / Concentration : 21.5->46 mg/L
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>LC0</td>
<td></td>
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<td></td>
</tr>
<tr>
<td>LC0 for 96 hours = 21.5 mg/L. (Nominal concentration).</td>
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<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

| LC100 |        |      |       |     |                                |
| LC100 for 96 hours > 46 mg/L. (Nominal concentration). |

References

**Primary Reference**: #URBSF*

**Secondary Reference**: !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

**End Point**: AQUATIC TOXICITY

**Chemical Name**: 6-Octen-1-yn-3-ol, 3,7-dimethyl-

**CAS Number**: 29171-20-8

**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>FISH</td>
<td>AQ</td>
<td>FRESH</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Species/strain/system**: Goldfish (Carassius auratus)

Test Method and Conditions

**Test method description**: Test methods are not specified. GLP: no

Exposure

**Dose / Concentration**: 20 ug/L

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>TLV</td>
<td>BEHAV</td>
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<td></td>
<td></td>
</tr>
</tbody>
</table>

TLV = 20 ug/L. (Equilibrium and spontaneous or reflex activity is disturbed.)
References

Primary Reference : APFRAD
Binet, M. P. Annales Pharmaceutiques Francaises, 30(10), 653-658, (1972)

Secondary Reference : !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point : AQUATIC TOXICITY
Chemical Name : 6-Octen-1-yn-3-ol, 3,7-dimethyl-
CAS Number : 29171-20-8
Study type : LAB

Test Subject

Organism Medium Specification Route Lifestage Sex Number exposed Number controls
MCR
Species/strain/system : Bacteria (Pseudomonas putida)

Test Substance

Purity Grade : &ge;99%

Test Method and Conditions

Test method description : DIN 38412 T.8; Growth Inhibition Test; GLP: no

Exposure

Dose / Concentration : 1800-2000 mg/L
Exposure comments : Doses of 1900 mg/L were also tested.

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>POPUL</td>
<td>EC10</td>
<td></td>
<td>------</td>
<td></td>
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<tr>
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<td></td>
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<tr>
<td></td>
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<td>EC10: 1800 mg/L</td>
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</tr>
<tr>
<td>POPUL</td>
<td>EC50</td>
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<td></td>
<td>------</td>
<td></td>
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</tr>
<tr>
<td></td>
<td></td>
<td>EC50: 1900 mg/L</td>
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<td></td>
</tr>
<tr>
<td>POPUL</td>
<td>EC90</td>
<td></td>
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<td>------</td>
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<tr>
<td></td>
<td></td>
<td>EC90: &gt;2000 mg/L</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Aquatic Toxicity

References

Primary Reference: #URBSF*

Secondary Reference: !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point: AQUATIC TOXICITY
Chemical Name: 6-Octen-1-yn-3-ol, 3,7-dimethyl-
CAS Number: 29171-20-8
Study type: LAB

Test Subject

Organism Medium Specification Route Lifestage Sex Number exposed Number controls
MCR AQ SLUDG
Species/strain/system: Activated sludge

Test Substance

Purity Grade: 99%

Test Method and Conditions

Test method description: ISO 8192. Test for inhibition of oxygen consumption by activated sludge;
GLP: no

Exposure

Exposure Type: ACUTE
Exposure Period: 30 mi
Dose / Concentration: 160 mg/L

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>POPUL</td>
<td>EC20</td>
<td>-----</td>
<td>------</td>
<td>-----</td>
<td>--------------------------------</td>
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<td>INHIB</td>
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<td></td>
<td></td>
<td>OXY</td>
</tr>
</tbody>
</table>
EC20 for 30 minutes: ca. 160 mg/L.

References

Primary Reference: #URBSF*
BASF. BASF, Unpublished Report, (1990)

Secondary Reference: !SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)