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# I U C L I D

## Data Set

**Existing Chemical** : ID: 4223-03-4  
**EINECS Name** : 2-Propenamide, N-(1,1,3,3-tetramethylbutyl)-  
**EC No.** : 224-169-7  
**Molecular Formula** : C11H21NO

**Producer related part**  
**Company** : National Starch and Chemical Company  
**Creation date** : 17.10.2002

**Substance related part**  
**Company** : National Starch and Chemical Company  
**Creation date** : 17.10.2002

**Status** :  
**Memo** : High Production Volume Challenge Program

**Printing date** : 16.12.2002  
**Revision date** :  
**Date of last update** : 16.12.2002

**Number of pages** : 8

**Chapter (profile)** : Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2

**Reliability (profile)** : Reliability: without reliability, 1, 2, 3, 4

**Flags (profile)** : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

## 2. Physico-Chemical Data

Id 4223-03-4

Date 18.12.2002

### 2.1 MELTING POINT

Value : 55 - 60 °C  
Sublimation :  
Method : other  
Year :  
GLP : no  
Test substance : as prescribed by 1.1 - 1.4  
  
Remark : No other details are available.  
Reliability : (4) not assignable  
05.11.2002

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### 2.2 BOILING POINT

### 2.4 VAPOUR PRESSURE

### 2.5 PARTITION COEFFICIENT

#### 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water  
Value : < .1 g/l at °C  
pH value :  
concentration : at °C  
Temperature effects :  
Examine different pol. :  
pKa : at 25 °C  
Description :  
Stable :  
Deg. product :  
Method : other  
Year :  
GLP : no  
Test substance : as prescribed by 1.1 - 1.4  
  
Remark : No other details are available.  
Reliability : (4) not assignable  
13.12.2002

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### 3. Environmental Fate and Pathways

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#### 3.1.1 PHOTODEGRADATION

##### DIRECT PHOTOLYSIS

Half-life t<sub>1/2</sub> : 7.6 hour(s)  
Degradation : % after  
Quantum yield :  
Deg. product :  
Method : other (calculated): AOPWIN v 1.90  
Year : 2002  
GLP : no  
Test substance : as prescribed by 1.1 - 1.4

Remark : The photodegradation was estimated using the AOPWIN module of EPIWIN v 3.10 as 7.6 hours assuming a 12 hour day and a hydroxyl concentration of 1.5x10<sup>6</sup>/cm<sup>3</sup>.

05.11.2002

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#### 3.1.2 STABILITY IN WATER

#### 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

#### 3.5 BIODEGRADATION

## 4. Ecotoxicity

Id 4223-03-4  
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4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

## 5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

**Robust Summary *in-vitro* dermal absorption of 2-Propenamide, *N*-(1,1,3,3,-tetramethylbutyl)- through Human and Rat Epidermis**

<b>Test substance</b>	2-Propenamide, <i>N</i> -(1,1,3,3,-tetramethylbutyl)
Remarks	Purity 99.73% w/w
<b>Method</b>	Draft OECD dermal absorption 1996
Test type	<i>in-vitro</i> dermal absorption
GLP	Yes
Year	1998
<b>Method</b>	A static glass diffusion assay design, using male rat epidermis and female human abdominal epidermis based on the then current draft OECD protocol was used. Both rat and human epidermal membranes had their subcutaneous fat removed and were frozen before use. The integrity of the epidermal membranes was confirmed by measurement of their electrical resistance. 50% aqueous ethanol was used as the receptor fluid and was analysed by GLC. (LOQ 3 µg/mL).
<b>Test Conditions</b>	
Species	Rat, Human
Strain	Human: Not applicable. Rat: Wistar
Sex	Human: Female Rat: Male
Cell type	Epidermal membrane (whole tissue)
Age	Human: Not stated Rat: 28 days
Number of animals/donors	6 samples (3 donors, each in duplicate) for each species
Route	Dermal, unoccluded
Vehicle	None, applied directly
Doses	10 mg/cm <sup>2</sup> , equivalent to 24.4 mg
Statistical Method	Not applicable
<b>Results</b>	The concentration of test chemical in the 50% aqueous ethanol receptor fluid was sampled at 6, 8, 10 and 24 hours after dosing and determined by gas-liquid chromatography. For human epidermis, the amounts absorbed at less than ten hours were at or below the limit of quantification (5 µg/cm <sup>2</sup> ) increasing to a maximum of 9.4 µg/cm <sup>2</sup> at 24 hours. Over the 6-24 hour exposure period, the mean absorption rate was 0.522 µg/cm <sup>2</sup> /hr. The mass balance mean percentage recovered was 90%. Most of the dose, 85.7% (mean percentage) was recovered by mild skin washing, whereas 0.1% was detected in the epidermal membrane. For rat epidermis, the mean absorption rate was 1.386 µg/cm <sup>2</sup> /hr. The mass balance mean percentage recovered was 90.6%. Again, most of the dose, 90.6% (mean percentage) was recovered by mild skin washing but no chemical was recovered from the epidermal membrane. 2-Propenamide, <i>N</i> -(1,1,3,3,-tetramethylbutyl)- is considered to have a low rate of dermal penetration.
<b>Conclusions</b>	The dermal absorption of 2-Propenamide, <i>N</i> -(1,1,3,3,-tetramethylbutyl)- is low.
<b>Reliability</b>	(1) valid without restriction

## 5.1.1 ACUTE ORAL TOXICITY

## 5. Toxicity

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### 5.1.2 ACUTE INHALATION TOXICITY

### 5.1.3 ACUTE DERMAL TOXICITY

### 5.1.4 ACUTE TOXICITY, OTHER ROUTES

### 5.4 REPEATED DOSE TOXICITY

### 5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test  
System of testing : Salmonella typhimurium TA98, TA100, TA1535, TA1537, E. coli WP2urvA  
Test concentration : 0, 33.3, 100, 333, 1000, 3330, 5000 µg/plate  
Cycotoxic concentr. : 5000 µg/plate  
Metabolic activation : With and without  
Result : Negative  
Method : OECD Guide-line 471  
Year : 1998  
GLP : Yes  
Test substance : As prescribed by 1.1 - 1.4

Remark : Metabolic activation:  
Arochlor induced Rat liver S9.

Statistical methods:  
Mean number of revertants and standard deviations were calculated.  
Various criteria were established to constitute a valid assay and a positive response was indicated by a 2-3 fold increase in mean revertant number dependent on the bacterial tester strain.

Positive controls:  
Benzo[a]pyrene, 2-aminoanthracene, 2-nitrofluorene, sodium azide, 2-aminoanthracene, ICR-191, and 4-nitroquinoline-N-oxide) were run concurrently. DMSO was used as a vehicle control.

Reliability : (1) valid without restriction  
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Type : Mammalian cell gene mutation assay  
System of testing : L5178Y mouse lymphoma cells  
Test concentration : With metabolic activation: 0, 25, 100, 200, 300, 400, 500 µg/mL.  
Without metabolic activation: 0, 50, 100, 200, 300, 400, 500, 600 µg/mL  
Cycotoxic concentr. : Approximately 500 µg/mL  
Metabolic activation : With and without  
Result : Negative  
Method : OECD Guide-line 476  
Year : 1998  
GLP : Yes  
Test substance : As prescribed by 1.1 - 1.4

Remark : Metabolic activation:  
Arochlor induced Rat liver S9 plus sodium NADP and isocitrate.

Statistical methods:  
A positive response was considered as a mean mutant frequency twice the

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background mutant frequency.

Positive controls:

Methylmethanesulfonate and Methylcholanthrene. DMSO was used as a vehicle control.

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

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(4)

### 5.6 GENETIC TOXICITY 'IN VIVO'

**Type** : Micronucleus assay  
**Species** : Mouse  
**Sex** : Male  
**Strain** : CD-1  
**Route of admin.** : Oral, gavage  
**Exposure period** : 24 hours  
**Doses** : 175, 350, 700 mg/kg  
**Result** : Negative  
**Method** : OECD Guide-line 474  
**Year** : 1998  
**GLP** : Yes  
**Test substance** : As prescribed by 1.1 - 1.4

**Remark** : Positive control:  
Cyclophosphamide. Corn oil was used as a vehicle control.

Statistical methods: Assay data analysis by ANOVA. Statistically significant ( $p < 0.05$ ) differences were investigated using a Dunnett's t-test. Analyses were performed separately for each sampling time.

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

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### 5.8.1 TOXICITY TO FERTILITY

### 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

## 9. References

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- (2) National Starch and Chemical Company
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- (4) National Starch and Chemical Company. Unpublished Report. Mutagenicity test on N-tert-Octylacrylamide in the L5178Y TK +/- Mouse Lymphoma Forward Mutation Assay with a confirmatory Assay. Covance Inc, Study No.:19301-0-431OECD, (1998)
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- (6) National Starch and Chemical Company. Unpublished. In-Vitro Absorption of N-tert-Octylacrylamide through Human and Rat Epidermis. Central Toxicology Laboratory. Report No CTL/P/5922. (1998)