

# I U C L I D

# D a t a s e t

Existing Chemical            Substance ID: 123-54-6  
CAS No.                      123-54-6  
EINECS Name                pentane-2,4-dione  
EINECS No.                 204-634-0  
Molecular Formula         C5H8O2

Dataset created by:        EUROPEAN COMMISSION - European Chemicals Bureau

This dossier is a compilation based on data reported by the European Chemicals Industry following 'Council Regulation (EEC) No. 793/93 on the Evaluation and Control of the Risks of Existing Substances'. All (non-confidential) information from the single datasets, submitted in the IUCLID/HEDSET format by individual companies, was integrated to create this document.

The data have not undergone any evaluation by the European Commission.

Creation date:              18-FEB-2000

Number of Pages:          56

Chapters:                  all

Edition:                    Year 2000 CD-ROM edition

Flags:                      non-confidential

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European Chemicals Bureau

**1.0.1 OECD and Company Information**

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**1.0.2 Location of Production Site**

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**1.0.3 Identity of Recipients**

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**1.1 General Substance Information**

Substance type: organic  
Physical status: liquid

**1.1.1 Spectra**

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**1.2 Synonyms**

2,4-dioxopentane

Source: Wacker - Chemie GmbH Burghausen

2-propanone, acetyl

Source: Wacker - Chemie GmbH Burghausen

acetoacetone

Source: Wacker - Chemie GmbH Burghausen

Acetylaceton

Source: BRENNTAG Chemiepartner GmbH Mülheim

acetylacetone

Source: Wacker - Chemie GmbH Burghausen

diacetylmethane

Source: Wacker - Chemie GmbH Burghausen

**1.3 Impurities**

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**1.4 Additives**

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**1.5 Quantity**

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### **1.6.1 Labelling**

**Labelling:** as in Directive 67/548/EEC  
**Symbols:** Xn  
D  
**Specific limits:** yes  
**R-Phrases:** (10) Flammable  
(22) Harmful if swallowed  
**S-Phrases:** (2) Keep out of reach of children  
(21) When using do not smoke  
(23) Do not breathe ...  
(24/25) Avoid contact with skin and eyes

### **1.6.2 Classification**

**Classification:** as in Directive 67/548/EEC  
**Class of danger:** corrosive  
**R-Phrases:** (22) Harmful if swallowed  
  
**Classification:** as in Directive 67/548/EEC  
**Class of danger:**  
**R-Phrases:** (10) Flammable

### **1.7 Use Pattern**

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#### **1.7.1 Technology Production/Use**

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### **1.8 Occupational Exposure Limit Values**

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### **1.9 Source of Exposure**

**Remark:** Die Herstellung erfolgt in einem geschlossenen System durch thermische Umlagerung von Isopropenylacetat. Die Abgase werden zentral erfaßt und verbrannt.  
**Source:** Wacker - Chemie GmbH Burghausen

#### **1.10.1 Recommendations/Precautionary Measures**

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#### **1.10.2 Emergency Measures**

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### **1.11 Packaging**

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**1.12 Possib. of Rendering Subst. Harmless**

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**1.13 Statements Concerning Waste**

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**1.14.1 Water Pollution**

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**1.14.2 Major Accident Hazards**

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**1.14.3 Air Pollution**

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**1.15 Additional Remarks**

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**1.16 Last Literature Search**

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**1.17 Reviews**

-

**1.18 Listings e.g. Chemical Inventories**

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**2.1 Melting Point**

**Value:** = -23.5 degree C  
**Method:** other  
**GLP:** no data  
**Source:** Wacker - Chemie GmbH Burghausen (1)

**Value:** = -23.3 degree C  
**Method:** other  
**GLP:** no data  
**Source:** Wacker - Chemie GmbH Burghausen (2)

**Value:** = -23.2 degree C  
**Method:** other  
**GLP:** no data  
**Source:** Wacker - Chemie GmbH Burghausen (3)

**Value:** = -23 degree C  
**Method:** other  
**GLP:** no data  
**Source:** Wacker - Chemie GmbH Burghausen (4) (5) (6)

**2.2 Boiling Point**

**Value:** = 139 degree C at 1013 hPa  
**Method:** other  
**GLP:** no data  
**Source:** Wacker - Chemie GmbH Burghausen (3)

**Value:** = 140 degree C  
**Method:** other  
**GLP:** no data  
**Source:** Wacker - Chemie GmbH Burghausen (7)

**Value:** = 140.4 degree C  
**Method:** other  
**GLP:** no data  
**Source:** Wacker - Chemie GmbH Burghausen (8)

**Value:** = 140.5 degree C  
**Method:** other  
**GLP:** no data  
**Source:** Wacker - Chemie GmbH Burghausen (9) (1)

### 2.3 Density

**Type:** density  
**Value:** = .9728 g/cm<sup>3</sup> at 20 degree C  
**Method:** other  
**GLP:** no data  
**Source:** Wacker - Chemie GmbH Burghausen (9)

**Type:** relative density  
**Value:** = .975 g/cm<sup>3</sup> at 20 degree C  
**Method:** other  
**GLP:** no data  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** relative to the density of water at 4 degree C. (8)

**Type:** relative density  
**Value:** = .9753 g/cm<sup>3</sup> at 20 degree C  
**Method:** other  
**GLP:** no data  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** relative to the density of water at 20 degree C. (1)

**Type:** relative density  
**Value:** = .9721 g/cm<sup>3</sup> at 25 degree C  
**Method:** other  
**GLP:** no data  
**Remark:** relative to the density of water at 4 degree C.  
**Source:** Wacker - Chemie GmbH Burghausen (10)

**Type:** density  
**Value:** = .976 g/cm<sup>3</sup>  
**Method:** other  
**GLP:** no data  
**Source:** Wacker - Chemie GmbH Burghausen (3)

#### 2.3.1 Granulometry

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### 2.4 Vapour Pressure

**Value:** = 8.5 hPa at 20 degree C  
**Method:** other (measured)  
**GLP:** no data  
**Source:** Wacker - Chemie GmbH Burghausen (9) (7)

**Value:** = 20 hPa at 30 degree C  
**Method:** other (measured)  
**GLP:** no data  
**Source:** Wacker - Chemie GmbH Burghausen (9)

**Value:** = 50 hPa at 50 degree C  
**Method:** other (measured)  
**GLP:** no data  
**Source:** Wacker - Chemie GmbH Burghausen (9)

### 2.5 Partition Coefficient

**log Pow:** = .34  
**Method:** other (measured)  
**Year:**  
**GLP:** no data  
**Remark:** method: no further data available.  
results (1st reference): calculated values  
(3 different methods) 0.177, -1.62, 1.212.  
**Source:** Wacker - Chemie GmbH Burghausen (11) (12)

### 2.6.1 Water Solubility

**Value:** = 16 vol% at 20 degree C  
**Qualitative:** soluble  
**Method:** other  
**GLP:** no data  
**Source:** Wacker - Chemie GmbH Burghausen (8)

**Value:** = 16.6 other  
**Qualitative:** miscible  
**Method:** other  
**GLP:** no data  
**Remark:** unit in weight%.  
**Source:** Wacker - Chemie GmbH Burghausen (7)

### 2.6.2 Surface Tension

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**2.7 Flash Point**

**Value:** = 30 degree C  
**Type:** other  
**Method:** other  
**Year:**  
**GLP:** no data  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** type not specified. (7)

**Value:** = 34.5 degree C  
**Type:** other  
**Method:** other  
**Year:**  
**GLP:** no data  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** no data about type. (8)

**Value:** = 40.5 degree C  
**Type:** open cup  
**Method:** other  
**Year:**  
**GLP:** no data  
**Source:** Wacker - Chemie GmbH Burghausen (1)

**Value:** = 40.6 degree C  
**Type:** open cup  
**Method:** other  
**Year:**  
**GLP:** no data  
**Source:** Wacker - Chemie GmbH Burghausen (3)

**2.8 Auto Flammability**

**Value:** = 340 degree C  
**Method:** other  
**GLP:** no data  
**Source:** Wacker - Chemie GmbH Burghausen (9) (3)

**Value:** = 350 degree C  
**Method:** other  
**GLP:** no data  
**Source:** Wacker - Chemie GmbH Burghausen (8)

**2.9 Flammability**

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**2.10 Explosive Properties**

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**2.11 Oxidizing Properties**

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**2.12 Additional Remarks**

- Remark:** pKa 13.32+/-0.05 and ion-pairing constant pKNa 2.57+/-0.05  
for the TS in DMSO-d6 at 25 degree C.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** TS distilled (13)
- Remark:** vapor density 3.45  
**Source:** Wacker - Chemie GmbH Burghausen (3)
- Remark:** The chemical properties of the TS are determined by the  
keto-enol tautomerism that exists in all states of  
aggregation.  
**Source:** Wacker - Chemie GmbH Burghausen (8)
- Remark:** TS soluble in ethanol, chloroform, ether, benzene, acetone  
and glacial acetic acid.  
**Source:** Wacker - Chemie GmbH Burghausen (1)
- Remark:** converting factor: 1 mg/m3 = 0.240 ppm  
**Source:** Wacker - Chemie GmbH Burghausen (9)
- Remark:** Lower explosive limit in air 71 g/m3 at 20 degree C and  
1013 hPa.  
**Source:** Wacker - Chemie GmbH Burghausen (9)
- Remark:** Lower explosive limit < 1.7 Vol.-%.  
**Source:** Wacker - Chemie GmbH Burghausen (7)

**3.1.1 Photodegradation**

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**3.1.2 Stability in Water**

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**3.1.3 Stability in Soil**

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**3.2 Monitoring Data (Environment)**

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**3.3.1 Transport between Environmental Compartments**

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**3.3.2 Distribution**

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**3.4 Mode of Degradation in Actual Use**

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**3.5 Biodegradation**

**Type:** aerobic  
**Inoculum:** activated sludge, non-adapted  
**Concentration:** 100 mg/l related to Test substance  
**Degradation:** = 79 - 88 % after 28 day  
**Result:** readily biodegradable  
**Method:** OECD Guide-line 301 C "Ready Biodegradability: Modified MITI Test (I)"  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Source:** Wacker - Chemie GmbH Burghausen

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### **3.6 BOD5, COD or BOD5/COD Ratio**

**Method:** other

#### **C O D**

**Method:** other

**COD:** = 1787 mg/g substance

**Remark:** method: COD determined by the dichromate methode; inoculum at BOD5 bacterial strains from domestic sewage.  
validity: no further information available.

**Result:** ThOD for 1 g TS 1920 mg O<sub>2</sub>; 93.1% degradation at COD measurement;

BOD5: 1340 mg O<sub>2</sub>/g, 70% degradation (BOD related to ThOD).

**Source:** Wacker - Chemie GmbH Burghausen

**Test substance:** no data

(15)

### **3.7 Bioaccumulation**

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### **3.8 Additional Remarks**

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**AQUATIC ORGANISMS****4.1 Acute/Prolonged Toxicity to Fish**

**Type:** flow through  
**Species:** Carassius auratus (Fish, fresh water)  
**Exposure period:** 96 hour(s)  
**Unit:** mg/l **Analytical monitoring:** yes  
**LC50:** = 121  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: at least 5 concentrations plus control tested, GC analysis.  
result: 95% confidence limits: 111-133 mg/l.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** temperature 18.6-19.4 degree C; pH 7.65-7.94;  
DO 6.19-9.22 mg/l; hardness (CaCO3) 196 mg/l.  
**Test substance:** purity > 99%

(16)

**Type:** flow through  
**Species:** Ictalurus punctatus (Fish, fresh water)  
**Exposure period:** 96 hour(s)  
**Unit:** mg/l **Analytical monitoring:** yes  
**LC50:** = 106  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: at least 5 concentrations plus control tested, GC analysis.  
result: 95% confidence limits: 74.1-151 mg/l.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** temperature 18.6-19.4 degree C; pH 7.65-7.94;  
DO 6.19-9.22 mg/l; hardness (CaCO3) 196 mg/l.  
**Test substance:** purity > 99%

(16)

**Type:** flow through  
**Species:** Lepomis macrochirus (Fish, fresh water)  
**Exposure period:** 4 day  
**Unit:** mg/l **Analytical monitoring:** yes  
**LOEL :** = 81  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: lowest lethal concentration; ventilatory and cough frequency measured at LOEL.  
result: ventilatory frequency significantly elevated.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** Lake Superior water, total hardness 40-46 mg/l, pH 7.6-8.0, temperature 20 degree C; at least 4 bluegills per group.

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**Type:** flow through  
**Species:** Lepomis macrochirus (Fish, fresh water)  
**Exposure period:** 96 hour(s)  
**Unit:** mg/l **Analytical monitoring:** yes  
**LC50:** = 60.1  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: at least 5 concentrations plus control tested, GC analysis.  
result: LC50 and 95% confidence limits in mg/l:  
first exp. 66.9 (58.4-76.6), 2nd exp. 60.1 (50.3-71.8).  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** temperature 18.6-19.4 degree C; pH 7.65-7.94;  
DO 6.19-9.22 mg/l; hardness (CaCO3) 196 mg/l.  
**Test substance:** purity > 99%

(16)

**Type:** flow through  
**Species:** Pimephales promelas (Fish, fresh water)  
**Exposure period:** 96 hour(s)  
**Unit:** mg/l **Analytical monitoring:** yes  
**LC50:** = 104  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: chemical analysis by GLC.  
result: 95% confidence limits 98.3-110 mg/l; affected fishes became hyperactive and lost equilibrium prior to death.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** Lake Superior water; 25.2 degree C; 6.3 mg/l dissolved oxygen; hardness 46.5 mg/l CaCO3; pH 7.37; 25 fishes per group; 10 TS concentrations (28.5-295 mg/l) tested.  
**Test substance:** purity > 99%

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**Type:** flow through  
**Species:** Pimephales promelas (Fish, fresh water)  
**Exposure period:** 96 hour(s)  
**Unit:** mg/l **Analytical monitoring:** yes  
**LC50:** = 141  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: at least 5 concentrations plus control tested, GC analysis.  
result: LC50 and 95% confidence limits in mg/l:  
first exp. 141 (113-175), 2nd exp. 143 (131-157).  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** temperature 18.6-19.4 degree C; pH 7.65-7.94;  
DO 6.19-9.22 mg/l; hardness (CaCO3) 196 mg/l.  
**Test substance:** purity > 99%

(16)

**Type:** flow through  
**Species:** Pimephales promelas (Fish, fresh water)  
**Exposure period:** 96 hour(s)  
**Unit:** mg/l **Analytical monitoring:** yes  
**LC50:** = 142  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** result: 95% confidence limits 137-148 mg/l.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** flow through with 99% replacement in ca. 2 h; dissolved oxygen 7.57 mg/l; pH 7.32; 43.2 mg/l CaCO<sub>3</sub>; temperature 24-26 degree C; at least 4 concentrations plus control tested in duplicate; 10 28-34 days-old fishes per group.  
**Test substance:** purity > 99%

(19)

**Type:** flow through  
**Species:** Pimephales promelas (Fish, fresh water)  
**Exposure period:** 96 hour(s)  
**Unit:** mg/l **Analytical monitoring:** yes  
**LC50:** = 175  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** result: affected fish swam in a corkscrew/spiral pattern near the surface; hypoactive; lost equilibrium prior to death;  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** 17.7 degree C; dissolved oxygen 7.7 mg/l; pH 7.35; tank volume 24 l; total hardness 43.8 mg/l CaCO<sub>3</sub>; lake Superior water; analytical concentrations of the TS 29.2, 30.0, 43.1, 44.0, 63.3, 62.4 , 111, 112, 216, 219 mg/l; 10 fishes per group.  
**Test substance:** purity > 99%

(20)

**Type:** flow through  
**Species:** Salmo gairdneri (Fish, estuary, fresh water)  
**Exposure period:** 96 hour(s)  
**Unit:** mg/l **Analytical monitoring:** yes  
**LC50:** = 71.7  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: at least 5 concentrations plus control tested, GC analysis.  
result: LC50 and 95% confidence limits in mg/l: Rainbow trout 92.4 (85-100), 2nd experiment 71.7 (64.1-80-1).  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** temperature 10.9 degree C; pH 7.65-7.94; DO 6.19-9.22 mg/l; hardness (CaCO<sub>3</sub>) 196 mg/l.  
**Test substance:** purity > 99%

(16)

**Type:** flow through  
**Species:** other  
**Exposure period:** 96 hour(s)  
**Unit:** mg/l **Analytical monitoring:** yes  
**LC50:** = 151  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** test species: *Gambusia affinis*; at least 5 concentrations plus control tested, GC analysis.  
result: LC50 and 95% confidence limits in mg/l:  
first exp. 204 (177-234), 2nd exp. 151 (90.6-252).  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** temperature 18.6-19.4 degree C; pH 7.65-7.94;  
DO 6.19-9.22 mg/l; hardness (CaCO<sub>3</sub>) 196 mg/l.  
**Test substance:** purity > 99%

(16)

**Type:** flow through  
**Species:** other  
**Exposure period:** 96 hour(s)  
**Unit:** mg/l **Analytical monitoring:** yes  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: simultaneous species testing (5 fish species with crayfish and snail) in the same tank; tanks divided in several compartments; conc. analysis 4 times during exposure; 5 conc. tested (29.6-217 mg/l) plus control;  
result: LC50 and 95% confidence limits in mg/l:  
fathead minnow: 155 (111-217);  
rainbow trout: 71.6 (64.5-79.4);  
goldfish: 107 (93.5-123).  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** diluter flow rate 130 ml/min; 90% replacement in 6 h; 20 animals per group except crayfish (n=10); temperature 17.3 degree C; oxygen concentration 4.7-10.0 mg/l; lake superior water; total hardness 44.4 mg/kg; pH 7.1-7.8.

(21)

**Type:** other  
**Species:** Leuciscus idus melanotus (Fish, fresh water)  
**Exposure period:**  
**Unit:** mg/l **Analytical monitoring:**  
**LC0:** = 97  
**LC50:** = 116  
**LC100:** = 136  
**Method:** other  
**Year:** 1976 **GLP:** no data  
**Test substance:** no data  
**Remark:** method: according to "Deutsche Einheitsverfahren zur Wasser-, Abwasser-, Schlammuntersuchung. L15: Fischtest" in: Vom Wasser 46, 291-295 (1976).  
result: same results in a 2nd lab: 78 (LC0), 146 (LC50), 485 mg/l (LC100), respectively.  
**Source:** Wacker - Chemie GmbH Burghausen (22)

#### 4.2 Acute Toxicity to Aquatic Invertebrates

**Species:** Ceriodaphnia sp. (Crustacea)  
**Exposure period:** 48 hour(s)  
**Unit:** mg/l **Analytical monitoring:** no  
**EC50:** > 48.5  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: closed static bioassay; animals fedded;  
test species C. reticulata.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** total hardness (CaCO<sub>3</sub>) 45 mg/l; pH 7.2-7.4; Lake superior water; 5 animals per group; duplicate experiments. (23)

**Species:** Ceriodaphnia sp. (Crustacea)  
**Exposure period:** 48 hour(s)  
**Unit:** mg/l **Analytical monitoring:** no  
**EC50:** = 75  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: closed static bioassay; test species C. reticulata;  
result: 95% confidence limits 72-78 mg/l;  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** total hardness 240 mg/l; pH 8.0+/-0.3; aerated (before use)  
carbon-filtered well water; 23 degree C; 16 h photoperiod;  
10 animals per group; at least 5 concentrations;  
duplicated tests; nominal concentration; not aerated;  
mortality or immobility determined;  
**Test substance:** reagent grade (24)

**Species:** Daphnia magna (Crustacea)  
**Exposure period:** 24 hour(s)  
**Unit:** mg/l **Analytical monitoring:** no data  
**EC0:** = 12  
**EC50:** = 40  
**EC100:** = 90  
**Method:** other  
**Year:** **GLP:** no data

**Test substance:** no data  
**Remark:** method: closed static bioassay  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** 10 24-h-old animals per group; medium was tap water, saturated with oxygen, hardness 16 degree (German, pH 7.8-8.2, temperature 20 degree C, final oxygen concentration > 2 mg/l.

(25)

**Species:** Daphnia magna (Crustacea)  
**Exposure period:** 24 hour(s)  
**Unit:** mg/l **Analytical monitoring:** no data  
**EC0:** = 45  
**EC50:** = 100  
**EC100:** = 125  
**Method:** other  
**Year:** **GLP:** no data

**Test substance:** no data  
**Remark:** method: closed static bioassay  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** 24-h-old animals used; medium was chlorine free tap water, saturated with oxygen, hardness 16 degree (German), pH 7.6-7.7, temperature 20-22 degree C.

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**Species:** Daphnia magna (Crustacea)  
**Exposure period:** 48 hour(s)  
**Unit:** mg/l **Analytical monitoring:** no  
**EC50:** = 34.4  
**Method:** other  
**Year:** **GLP:** no data

**Test substance:** no data  
**Remark:** method: closed static bioassay; animals fed.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** total hardness (CaCO<sub>3</sub>) 45 mg/l; pH 7.2-7.4; Lake superior water; 5 animals per group; duplicate experiments.

(23)

**Species:** Daphnia magna (Crustacea)  
**Exposure period:** 48 hour(s)  
**Unit:** mg/l **Analytical monitoring:** yes  
**EC50:** = 47.6  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: closed static bioassay; at least 5 concentrations tested, GC analysis.  
result: 95% confidence limits 43.4-52.1 mg/l.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** 20 animals per group; temperature 19.1 degree C; pH 8.18; DO 7.66 mg/l.  
**Test substance:** purity > 99%

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**Species:** Daphnia magna (Crustacea)  
**Exposure period:** 48 hour(s)  
**Unit:** mg/l **Analytical monitoring:** no  
**EC50:** = 75  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: closed static bioassay.  
result: 95% confidence limits 72-78 mg/l;  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** total hardness (CaCO<sub>3</sub>) 240 mg/l; pH 8.0+/-0.3; aerated (before use); carbon-filtered well water; 23 degree C; 16 h photoperiod; 10 animals per group; at least 5 concentrations; duplicated tests; nominal concentration; not aerated during test; mortality or immobility determined;  
**Test substance:** reagent grade

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**Species:** Daphnia pulex (Crustacea)  
**Exposure period:** 48 hour(s)  
**Unit:** mg/l **Analytical monitoring:** no  
**EC50:** > 48.5  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: closed static bioassay; animals fed.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** total hardness (CaCO<sub>3</sub>) 45 mg/l; pH 7.2-7.4; Lake superior water; 5 animals per group; duplicate experiments.

(23)

**Species:** Daphnia pulex (Crustacea)  
**Exposure period:** 48 hour(s)  
**Unit:** mg/l **Analytical monitoring:** no  
**EC50:** = 75  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: closed static bioassay.  
result: 95% confidence limits 72-78 mg/l;  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** total hardness (CaCO<sub>3</sub>) 240 mg/l; pH 8.0+/-0.3; aerated  
(before use); carbon-filtered well water; 23 degree C;  
16 h photoperiod; 10 animals per group; at least  
5 concentrations; duplicated tests; nominal concentration;  
not aerated; mortality or immobility determined;  
**Test substance:** reagent grade

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**Species:** other aquatic arthropod  
**Exposure period:** 48 hour(s)  
**Unit:** mg/l **Analytical monitoring:** yes  
**EC50:** = 158  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** as prescribed by 1.1 - 1.4  
**Remark:** method: static bioassay in closed system;  
test organism: larvae of Tanytarsus dissimilis;  
at least 5 concentrations tested, GC analysis.  
result: 95% confidence limits 136-183 mg/l.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** 20 animals per group; temperature 20.6 degree C; 7.99;  
DO 4.04 mg/l.  
**Test substance:** purity > 99%

(16)

**Species:** other aquatic mollusc  
**Exposure period:** 96 hour(s)  
**Unit:** mg/l **Analytical monitoring:** yes  
**EC50:** = 155  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: flow through assay; species snail (Aplexa hypnorum);  
simultaneous species testing (5 fish species with crayfish  
and snail) in the same tank; tanks divided in several  
compartments; conc. analysis 4 times during exposure;  
5 conc. tested (29.6-217 mg/l) plus control;  
result: 95% confidence limits 111-217 mg/l  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** diluter flow rate 130 ml/min; 90% replacement in 6 h;  
20 animals per group except crayfish (n=10); lake superior  
water; temperature 17.3 degree C; pH 7.1-7.8; DO 4.7-  
10.0 mg/l; total hardness (CaCO<sub>3</sub>) 44.4 mg/kg.

(21)

**Species:** other aquatic crustacea  
**Exposure period:** 48 hour(s)  
**Unit:** mg/l **Analytical monitoring:** no  
**EC50:** > 48.5  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: closed static bioassay; test species Simocephalus  
vetulus; animals fed.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** total hardness (CaCO<sub>3</sub>) 45 mg/l; pH 7.2-7.4; Lake superior  
water; 5 animals per group; duplicate experiments.

(23)

**Species:** other aquatic crustacea  
**Exposure period:** 96 hour(s)  
**Unit:** mg/l **Analytical monitoring:** yes  
**EC50:** > 217  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: flow through assay; species crayfish (*Orconectes  
immunis*); simultaneous species testing (5 fish species with  
crayfish and snail *Aplexa hypnorum*) in the same tank; tanks  
divided in several compartments; conc. analysis 4 times  
during exposure; 5 conc. tested (29.6-217 mg/l) plus  
control;  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** diluter flow rate 130 ml/min; 90% replacement in 6 h;  
20 animals per group except crayfish (n=10); lake superior  
water; temperature 17.3 degree C; pH 7.1-7.8; DO 4.7-  
10.0 mg/l; total hardness (CaCO<sub>3</sub>) 44.4 mg/kg.

(21)

**Species:** other aquatic crustacea  
**Exposure period:** 96 hour(s)  
**Unit:** mg/l **Analytical monitoring:** yes  
**EC50:** = 388  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: flow-through bioassay with crayfish (*Orconectes  
immunis*); at least 5 concentrations tested, GC analysis.  
result: 95% confidence limits 322-467 mg/l; 2nd experiment  
LC50 631 (558-713) mg/l.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** temperature 11.0 degree C (2nd exp. 11.2); pH 7.72 (7.83);  
DO 8.77 (9.03) mg/l; mean body weight 0.52 g (1.18).  
**Test substance:** purity > 99%

(16)

**4.3 Toxicity to Aquatic Plants e.g. Algae**

**Species:** Scenedesmus quadricauda (Algae)  
**Endpoint:** growth rate  
**Exposure period:** 8 day  
**Unit:** mg/l **Analytical monitoring:** no data  
**TTC :** = 2.7  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: TTC= toxicity threshold concentration; closed static bioassay.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** TS dissolved in bidistilled water; neutral pH; vials shaken once daily;

(27) (28) (29)

**Species:** other algae  
**Endpoint:** other  
**Exposure period:** 24 hour(s)  
**Unit:** mg/l **Analytical monitoring:** no data  
**EC10:** = 100  
**EC50:** > 300  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:**  
**Remark:** method: static bioassay in closed system; inhibition of assimilation in multispecies batch cultures of green algae (chlorococcales, mainly Scenedesmus sp., not sterile); measurement of O<sub>2</sub>-production.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** temperature 20 degree C; light incubation: 3000 lx; controls incubated in darkness; 6 concentrations tested; duplicate trials.

(30)

**4.4 Toxicity to Microorganisms e.g. Bacteria**

**Type:** aquatic  
**Species:** Chilomonas paramecium (Protozoa)  
**Exposure period:** 48 hour(s)  
**Unit:** mg/l **Analytical monitoring:** no data  
**TTC :** = 62  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: cell multiplication inhibition test; TTC = toxicity threshold concentration.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** temperature 20 degree C; TS dissolved in distilled water; pH 6.9.

(31)

**Type:** aquatic  
**Species:** Entosiphon sulcatum (Protozoa)  
**Exposure period:** 72 hour(s)  
**Unit:** mg/l **Analytical monitoring:** no data  
**TTC :** = 11  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: cell multiplication inhibition test;  
TTC = toxicity threshold concentration.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** temperature 25 degree C; pH 6.9.

(32) (33) (29)

**Type:** aquatic  
**Species:** Microcystis aeruginosa (Bacteria)  
**Exposure period:** 8 day  
**Unit:** mg/l **Analytical monitoring:** no data  
**TTC :** = 8.5  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: cell multiplication inhibition test;  
TTC = toxicity threshold concentration.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** temperature 27 degree C; pH 7; vials shaken once daily.

(34) (27) (28)

**Type:** aquatic  
**Species:** Photobacterium phosphoreum (Bacteria)  
**Exposure period:** 5 minute(s)  
**Unit:** mg/l **Analytical monitoring:** no  
**EC50:** = 1050  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: Microtox test; measurement of the effective  
concentration that results in a 50% reduction of bacterial  
luminescence; nominal concentrations.  
**Source:** Wacker - Chemie GmbH Burghausen

(35)

**Type:** aquatic  
**Species:** Pseudomonas putida (Bacteria)  
**Exposure period:** 16 hour(s)  
**Unit:** mg/l **Analytical monitoring:** no data  
**TTC :** = 67  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: cell multiplication inhibition test;  
TTC = toxicity threshold concentration.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** TS dissolved in distilled water; pH 7.0; 25 degree C.

(29) (36)

**Type:** aquatic  
**Species:** Uronema parduzci (Protozoa)  
**Exposure period:**  
**Unit:** mg/l **Analytical monitoring:** no data  
**TTC :** = 5.9  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: cell multiplication inhibition test.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** no further information available.

(37)

**Type:** aquatic  
**Species:** other bacteria  
**Exposure period:** 15 minute(s)  
**Unit:** mg/l **Analytical monitoring:** no  
**EC50:** = 373  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: Microtox test according to Beckmann Instruments Inc., Microtox \* System Operating Manual, Fullerton, CA (1982).  
**Source:** Wacker - Chemie GmbH Burghausen

(38)

**Type:** other  
**Species:** other bacteria  
**Exposure period:**  
**Unit:** mg/l **Analytical monitoring:** no  
**EC10:** = 75  
**EC50:** = 110  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: oxygen consumption test.  
validity: no further information available.  
**Source:** Wacker - Chemie GmbH Burghausen

(30)

**4.5 Chronic Toxicity to Aquatic Organisms****4.5.1 Chronic Toxicity to Fish**

-

**4.5.2 Chronic Toxicity to Aquatic Invertebrates**

**Species:** other  
**Endpoint:** reproduction rate  
**Exposure period:** 7 day  
**Unit:** mg/l **Analytical monitoring:** no  
**EC50:** = 2.6  
**MATC :** < .87  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: static bioassay in closed system; test organism: Ceriodaphnia reticulata.  
result: EC50 95% confidence limits 1.6-4.1 mg/l; EC50 for mortality of adults > 8.7 mg/l (greater than highest concentration tested).  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** temperature 23 degree C; pH 8.0+/-0.3; carbon-filtered well water (aerated before use); total hardness (in CaCO3) 240 mg/l; 16 h photoperiod/day; 10 animals per group; at least 5 concentrations tested; duplicated tests; nominal concentrations; not aerated; renewal every second day; feeding every day.  
**Test substance:** reagent grade

(24)

**Species:** Daphnia magna (Crustacea)  
**Endpoint:** reproduction rate  
**Exposure period:** 14 day  
**Unit:** mg/l **Analytical monitoring:** no  
**LOEC:** = .5  
**EC50:** = 6.5  
**MATC :** = 6.5  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: static bioassay in closed system.  
result: EC50 95% confidence limits 5-9 mg/l; EC50 for mortality of adults: 6.5 mg/l.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** temperature 23 degree C; pH 8.0+/-0.3; total hardness (as CaCO3) 240 mg/l; carbon-filtered well water (aerated before use); 16 h photoperiod/day; 10 animals per group; at least 5 TS concentrations; duplicated tests; nominal concentrations; not aerated; renewal every 2nd day; feeding every day;  
**Test substance:** reagent grade

(24)

**Species:** Daphnia pulex (Crustacea)  
**Endpoint:** reproduction rate  
**Exposure period:** 14 day  
**Unit:** mg/l **Analytical monitoring:** no  
**EC50:** = 1  
**MATC :** < .87  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: static bioassay in closed system.  
 result: EC50 95% confidence limits 0.2-1.7 mg/l; EC50 for mortality of adults: 4.7 mg/l.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** temperature 23 degree C; pH 8.0+/-0.3; carbon-filtered well water (aerated before use); total hardness (in CaCO3) 240 mg/l; 16 h photoperiod/day; 10 animals per group; at least 5 concentrations; duplicated tests; nominal concentrations; not aerated; renewal every 2nd day; feeding every day.  
**Test substance:** reagent grade

(24)

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Soil Dwelling Organisms

-

### 4.6.2 Toxicity to Terrestrial Plants

-

### 4.6.3 Toxicity to other Non-Mamm. Terrestrial Species

**Species:** other  
**Endpoint:** mortality  
**Expos. period:** 96 hour(s)  
**Unit:** other  
**LC50:** = 74  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: flow-through test; TS concentration checked by GC analysis; species: Rana catesbiana (tadpole).  
 result: unit in mg/l; 2nd experiment LC50 156 mg/l.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test condition:** temperature 21.5 (16.8) degree C; pH 8.03 (7.85); DO 5.95 (7.80) mg/l; water replacement time 3-8 h.  
**Test substance:** purity>99%

(16)

### 4.7 Biological Effects Monitoring

-

#### 4.8 Biotransformation and Kinetics

-

#### 4.9 Additional Remarks

**Remark:** the carboxylation of phosphoenolpyruvate to form oxalacetate is catalyzed by the chicken liver enzyme phosphoenolpyruvate carboxykinase; the TS inactivated this enzyme with a second order rate constant of  $0.36 \pm 0.025$  M/min.

**Source:** Wacker - Chemie GmbH Burghausen

**Test substance:** no data

(39)

**Remark:** method: sea urchin embryos (*Arbacia punctulata*) were incubated 1 h after fertilization with the TS for 3 h and tritiated thymidine added last 2 h;  
result: the incorporation of thymidine was inversely related to the TS concentration; EC50 of 2 different trials: 206 mg/l (95% confidence limits 68-561 mg/l), 169 mg/l (81-240 mg/l).

**Source:** Wacker - Chemie GmbH Burghausen

**Test substance:** no data

(40)

**Remark:** method: sea urchin embryos (*Arbacia punctulata*) were incubated at fertilization with the TS for 5 h and increase in DNA measured by fluorometric determination  
result: the DNA increase was inversely related to the TS concentration; EC50 21.3 mg/l (95% confidence limits 14.6-31.1 mg/l)

**Source:** Wacker - Chemie GmbH Burghausen

**Test substance:** no data

(41)

**Remark:** method: 2 lipases secreted from *Rhodotorula pilimanae* were incubated with 3 mM TS.  
result: activity of the enzymes decreased to 74 and 57% of control values.

**Source:** Wacker - Chemie GmbH Burghausen

**Test substance:** no data

(42)

**Remark:** method: a) sea urchin embryos (*Arbacia punctulata*) were incubated at fertilization with the TS for 4 h and tritiated thymidine added last 2 h; b) sperm cells of the same species were incubated for 1 h at 20 degree C with TS and degree of fertilization measured thereafter.

result: a) the incorporation of thymidine (DNA-synthesis) was inversely related to the TS concentration; EC50 105.4 mg/l (95% confidence limits 56.5-170.3 mg/l); b) EC50 for sperm cell toxicity 0.9 mg/l (95% confidence limit 0.8-1.1 mg/l).

**Source:** Wacker - Chemie GmbH Burghausen

**Test substance:** no data

(38)

**Remark:** method: homogeneous preparations of the Escherichia coli 2-keto-4-hydroxygluterate aldolase were incubated for 0-90 min at 37 degree C with 10 mM TS.  
result: TS inhibited time-dependent the activity of the bacterial enzyme.

**Source:** Wacker - Chemie GmbH Burghausen

**Test substance:** no data

(43)

**Remark:** method: sea urchin embryos (Arbacia punctulata) were incubated with TS a) 1 h before fertilization, b) at fertilization or c) 1 h after fertilization; all exposures continued through the period of tritiated thymidine incorporation (4 h after fertilization).  
result: the incorporation of thymidine was inversely related to the TS concentration; EC50 and 95% confidence limits in mg/l: a) 105.4 (56.4-170.2), b) 60.8 (4.4-160.3), c) 395.0 (222.3-886.4).

**Source:** Wacker - Chemie GmbH Burghausen

**Test substance:** no data

(44)

**Remark:** method: dihydrofolate reductase from an amethopterin-resistant strain of Lactobacillus casei was incubated with 200 mM TS at 30 degree C for 0-140 min; activity of the enzyme measured periodically.  
result: the enzyme was time-dependent inactivated by the TS (activity 5% after 140 min); inactivation was concomitant with the modification of three lysyl residues.

**Source:** Wacker - Chemie GmbH Burghausen

**Test substance:** purity > 99%

(45)

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

**Type:** LD50  
**Species:** rat  
**Sex:**  
**Number of Animals:**  
**Vehicle:**  
**Value:** = 760 mg/kg bw  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: 5 male or 5 female Hilltop-Wistar rats per group; 4 doses tested; 14 d postdosing observation period; undiluted TS was given.  
results: LD50 in female rats 570 mg/kg; deaths occurred 2-24 h after application; signs of toxicity seen at doses of 490 mg/kg and more: ataxia, prostration, lachrymation, tremor, twitching movements and convulsions; no effects determined at gross pathology of animals that died and sacrificed survivors.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** purity>99%

(46)

**Type:** LD50  
**Species:** rat  
**Sex:**  
**Number of Animals:**  
**Vehicle:**  
**Value:** = 1000 mg/kg bw  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: 6 male Wistar rats per group; at least 4 doses tested; postdosing observation period 14 d.  
result: respective hazard of formaldehyde.  
**Source:** Wacker - Chemie GmbH Burghausen

(47)

**Type:** LD50  
**Species:** rat  
**Sex:**  
**Number of Animals:**  
**Vehicle:**  
**Value:** = 800 mg/kg bw  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** results: male rats; 95% confidence limits 540-1184 mg/kg; weakness and prostration observed.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** purity ca. 100%

(48)

**Type:** LD50  
**Species:** rat  
**Sex:**  
**Number of Animals:**  
**Vehicle:**  
**Value:**  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: data of a program to monitor the repeatability of LD50 data and to assay annual production material in biological tests.  
results: LD50 (in mg/kg) in the year 1944 970, 1952 1120, 1953 930, 1954 1220, 1955 1120, 1956 940, 1957 1120, 1958 1160, 1959 1450, 1960 960, 1961 1120, 1962 890, 1964 1410.  
validity: no further information available.  
**Source:** Wacker - Chemie GmbH Burghausen

(49)

**Type:** LD50  
**Species:** rat  
**Sex:**  
**Number of Animals:**  
**Vehicle:**  
**Value:** = 970 mg/kg bw  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: male albino rats.  
results: rapid death with marked narcosis due to paralysis of respiratory center.  
validity: no further information available.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** TS contained acetic acid.

(50)

**Type:** LD50  
**Species:** mouse  
**Sex:**  
**Number of Animals:**  
**Vehicle:**  
**Value:** = 951 mg/kg bw  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** results: male mice; 95% confidence limits 677-1336 mg/kg; weakness and prostration observed.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** purity ca. 100%

(48)

**5.1.2 Acute Inhalation Toxicity**

**Type:** LC50  
**Species:** rat  
**Sex:**  
**Number of Animals:**  
**Vehicle:**  
**Exposure time:** 4 hour(s)  
**Value:** = 1224 ppm  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: groups of 5 male and 5 female Hilltop-Wistar rats were exposed to 600, 930, 1260 and 1500 ppm; TS concentration concurrently analysed; postexposure period 14 d; body weight determined at 0, 7 and 14 d postexposure; for determination of LT50, groups of 5 male and 5 female rats exposed for various periods to TS saturated atmosphere.  
  
results: LC50 determined for combined male and female rats; LC50 for female rats 1250 ppm; deaths occurred during exposure or first 24 h after exposure (1 exception on day 3); signs of toxicity: periocular, perinasal and perioral wetness and encrustation, mouth and abdominal breathing, tremor, ataxia, no tail and toe pinch reflex; body weight unaffected; necropsy of rats that died: red lungs, dark livers, gas-filled stomachs (no effects on sacrificed survivors); LT 50 for male rats 52 min (average concentration 7060 ppm) and 55 min for female rats (average conc. 7912 ppm).  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** purity 99.42% before the study and 98.74% after completion. (46)

**Type:** other  
**Species:** rat  
**Sex:**  
**Number of Animals:**  
**Vehicle:**  
**Exposure time:** 30 minute(s)  
**Value:**  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** result: max. time for no death of 6 male rats exposed to saturated vapor.  
**Source:** Wacker - Chemie GmbH Burghausen (47)

**Type:** other  
**Species:** rat  
**Sex:**  
**Number of Animals:**  
**Vehicle:**  
**Exposure time:** 4 hour(s)  
**Value:** = 1000 ppm  
**Method:** other  
**Year:** **GLP:** no  
**Test substance:** no data  
**Remark:** method: 6 male or female Sherman rats exposed to nominal concentration; post exposure observation period 14 days.  
result: 2-4 rats died.  
validity: no further information available.  
**Source:** Wacker - Chemie GmbH Burghausen

(51)

**Type:** other  
**Species:** rat  
**Sex:**  
**Number of Animals:**  
**Vehicle:**  
**Exposure time:**  
**Value:** = 1000 ppm  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** result: 2/6 rats died in 2 h and 4/6 died in 4 h; rats exposed to saturated vapor all died within 1 h.  
validity: no further information available.  
**Source:** Wacker - Chemie GmbH Burghausen

(50) (52)

**Type:** other  
**Species:** rat  
**Sex:**  
**Number of Animals:**  
**Vehicle:**  
**Exposure time:** 4 hour(s)  
**Value:**  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: 10 male and 10 female Fischer 344 rats exposed to 1265 or 1811 ppm; 5 male and 5 female exposed to air alone for each exposure group; surviving rats sacrificed after a 4-day post exposure observation period;  
results: 2/20 (1 m and 1 f) rats died immediately following 1265 ppm exposure and 6 m and 8 f died during or within 5 h following the 1811 ppm exposure; clinical signs: blepharospasm, lacrimation, abdominal breathing, urogenital wetness, decreased activity, encrustation around eyes and nose; survivors of 1811 ppm group with eye opacities; significantly decreased absolute body weight and body weight

gain for both sexes on day 4; the only microscopical lesions were keratitis and lymphoid atrophy in a few 1811 ppm survivors; no degenerative lesions in the brain of rats dying from or surviving exposure of the TS.

**Source:** Wacker - Chemie GmbH Burghausen

**Test substance:** purity > 99%

(53)

### 5.1.3 Acute Dermal Toxicity

**Type:** LD50

**Species:** rabbit

**Sex:**

**Number of  
Animals:**

**Vehicle:**

**Value:** = 1370 mg/kg bw

**Method:** other

**Year:**

**GLP:** no data

**Test substance:** other TS

**Remark:** method: undiluted TS applied on the shaved dorsal skin (25 cm<sup>2</sup>) of 3-5 male or female New Zealand White rabbits/group; occlusive contact for 24 h; 14 d postapplication period; 5 doses tested.

result: LD50 in female rabbits 790 mg/kg; death occurred within 1-24 h after application; signs of toxicity at 970 mg/kg or more: dilated pupils, salivation and convulsions (high dose); local erythema, edema and necrosis (persisted for 1-7 d) and scab formation at day 14; no effect on body weight in survivors; dead animals showed red mottled lungs, patchy congestion of tracheal mucosa, and a few stomachs with superficial black foci at necropsy.

**Source:** Wacker - Chemie GmbH Burghausen

**Test substance:** purity>99%

(46)

**Type:** LD50

**Species:** rabbit

**Sex:**

**Number of  
Animals:**

**Vehicle:**

**Value:** ca. 4870 mg/kg bw

**Method:** other

**Year:**

**GLP:** no data

**Test substance:** no data

**Remark:** method: rubber dam rabbit test with 24 h contact; TS undiluted.

validity: no further information available.

**Source:** Wacker - Chemie GmbH Burghausen

(50)

**Type:** LD50  
**Species:** guinea pig  
**Sex:**  
**Number of Animals:**  
**Vehicle:**  
**Value:** 9750 - 19500 mg/kg bw  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: occlusive wrap for 24 h.  
results: 4 animals receiving 20 ml/kg died within 24-72 h after application; absorption evident; moderate irritation. validity: no further information available.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** purity ca. 100%

(48)

#### **5.1.4 Acute Toxicity, other Routes**

**Type:** LD0  
**Species:** rat  
**Sex:**  
**Number of Animals:**  
**Vehicle:**  
**Route of admin.:** i.p.  
**Value:** = 300 mg/kg bw  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Source:** Wacker - Chemie GmbH Burghausen

(54)

**Type:** LD100  
**Species:** rat  
**Sex:**  
**Number of Animals:**  
**Vehicle:**  
**Route of admin.:** i.p.  
**Value:** = 400 mg/kg bw  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Source:** Wacker - Chemie GmbH Burghausen

(54)

## **5.2 Corrosiveness and Irritation**

### **5.2.1 Skin Irritation**

**Species:** rabbit

**Concentration:**

**Exposure:**

**Exposure Time:**

**Number of  
Animals:**

**PDII:**

**Result:** slightly irritating

**EC classificat.:**

**Method:** other

**Year:**

**GLP:** no data

**Test substance:** other TS

**Remark:** method: 0.5 ml undiluted TS applied on the dorsal skin of 6 New Zealand White rabbits for 4 h; occlusive; test site inspected 1 h and 1, 2, 3, 7 and 14 d after removal of the occlusive dressing.  
results: after 1 h slight erythema in 5, after 24 h in all rabbits; after 24 h slight edema in 5, moderate edema in 1 rabbit; after 3 d 3 animals with just detectable erythema, 1 with mild edema; except mild desquamation no effects at day 7.

**Source:** Wacker - Chemie GmbH Burghausen

**Test substance:** purity>99%

(46)

**Species:** rabbit

**Concentration:**

**Exposure:**

**Exposure Time:**

**Number of  
Animals:**

**PDII:**

**Result:** slightly irritating

**EC classificat.:**

**Method:** other

**Year:**

**GLP:** no data

**Test substance:** no data

**Remark:** method: covered, rabbit belly vesicant test; abraded and intact skin.

result: caused erythema but not edema.

**Source:** Wacker - Chemie GmbH Burghausen

(55)

**Species:** rabbit  
**Concentration:**

**Exposure:**  
**Exposure Time:**  
**Number of Animals:**  
**PDII:**  
**Result:** slightly irritating  
**EC classificat.:**  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: repeated skin applications, uncovered; 0.01 ml TS applied to the same spot on the clipped skin of the belly of 5 rabbits, 3 times a day for 3 days.  
results: after 3 applications 3/5 animals with moderate to marked capillary injection; after 6 applications moderate erythema in 1/5, moderate capillary injection on 3/5, 1/5 negative; same results after 9 applications.  
**Source:** Wacker - Chemie GmbH Burghausen

(55)

### 5.2.2 Eye Irritation

**Species:** rabbit  
**Concentration:**  
**Dose:**  
**Exposure Time:**  
**Comment:**  
**Number of Animals:**  
**Result:** slightly irritating  
**EC classificat.:**  
**Method:** Draize Test  
**Year:** 1944 **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: 6 New Zealand White rabbits tested; effects scored according to Draize (1944).  
result: 1 h after application conjunctiva redness 0.8, chemosis 0.7, discharge 1.3 and iris 0.3 (iritis); after 4 h 0.7, 0.7, 1.2, 0.2, respectively; all eyes healed by 24 h post instillation.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** purity>99%

(46)

**Species:** rabbit  
**Concentration:**  
**Dose:**  
**Exposure Time:**  
**Comment:**  
**Number of Animals:**  
**Result:** moderately irritating  
**EC classificat.:**  
**Method:** Draize Test  
**Year:** 1944 **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: 3 female Japanese white rabbits used.  
results: corneal involvement or irritation that persisted for more than 24 h but recovered within 21 d; authors classification moderate to severe irritant.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** reagent grade

(56)

**Species:** rabbit  
**Concentration:**  
**Dose:**  
**Exposure Time:**  
**Comment:**  
**Number of Animals:**  
**Result:**  
**EC classificat.:**  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: instillation of 0.1 (a) or 0.5 ml (b) TS, 2 samples.  
results: a) no corneal injury for the 1st and minor to moderate injury for the 2nd sample; b) both caused minor to moderate corneal injury.  
**Source:** Wacker - Chemie GmbH Burghausen

(55)

### 5.3 Sensitization

**Type:** Patch-Test  
**Species:** human  
**Number of Animals:**  
**Vehicle:**  
**Result:**  
**Classification:**  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: 12 control persons were tested with 100% TS.  
result: 3 showed no, 7 doubtful and 2 positive reaction to the TS after 24 h (not after 48 or 72 h).  
validity: possibly no sensitizing but irritating effect.  
**Source:** Wacker - Chemie GmbH Burghausen

(57)

**Type:** other  
**Species:** guinea pig  
**Number of Animals:**  
**Vehicle:**  
**Result:** ambiguous  
**Classification:**  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: standardized skin sensitization test.  
result: 1/5 animals with weak reaction.  
validity: no further information available.  
**Source:** Wacker - Chemie GmbH Burghausen

(48)

#### 5.4 Repeated Dose Toxicity

**Species:** rat **Sex:** male/female  
**Strain:** Fischer 344  
**Route of admin.:** inhalation  
**Exposure period:** 5 d, 2 d nonexposure period, followed by 4 d exposure (total 9 d exposure)  
**Frequency of treatment:** 6 h/d each day  
**Post. obs. period:** 1 d  
**Doses:** 0, 197, 418, 805 ppm  
**Control Group:** yes, concurrent vehicle  
**LOAEL:** = 197 ppm  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: 10 male and 10 female rats/group; TS concentration in the exposure chamber measured every 33 min during the exposure; clinical (every day prior, during and after exposure) and hematological (at sacrifice) parameters determined; necropsy; histopathology on high dose and control;  
**Result:** no mortality; significantly reduced body weight gain in both groups at 805 ppm and in male rats at 418 ppm; at 805 ppm significant leucocytosis in both sexes, increased mean corpuscular hemoglobin concentration and mean corpuscular hemoglobin in male rats; hematologic alteration not considered toxicologically significant; no treatment-related gross lesions; no effects on relative organ weights except thymus gland weights at 805 ppm in male and female rats (25-43% decrease); exposure-related inflammation of nasal mucosa in all rats, necrosis in 805 ppm rats and occasionally at 418 ppm; mild laryngitis in 2 males and mild vacuolization of the brain stem in 2 male rats of the 805 ppm-group.;  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** purity=99%

(58)

**Species:** rat **Sex:** male/female  
**Strain:** Fischer 344  
**Route of admin.:** inhalation  
**Exposure period:** 14 weeks  
**Frequency of treatment:** daily 6 h, 5 days per week  
**Post. obs. period:** 0 or 4 weeks  
**Doses:** 0, 101, 307, 650 ppm  
**Control Group:** yes, concurrent vehicle  
**NOAEL:** = 101 ppm  
**LOAEL:** = 307 ppm  
**Method:** other **GLP:** no data  
**Year:**  
**Test substance:** other TS  
**Remark:** method: 20 male and 20 female rats per group, with half being sacrificed at the end of exposure period and the remaining after a 4 week recovery period; 10 male rats added to control and high dose group for subsequent ultrastructural examination of sciatic nerves; TS concentration analysed every 33 min during the daily 6 h exposure; the following parameters were determined: clinical signs of toxicity (daily), ophtalmoscopy of the eye (before and after exposure), neurobehavior screen (monthly before, during and after exposure), body weight (weekly during the study and before sacrifice), food and water consumption for 14 h in metabolic cages during the last exposure week (urine samples taken), urine chemistry (n=10 each group), serum chemistry and hematology of blood samples collected at the end of exposure or the 4-week recovery; gross pathology at termination in all groups; histopathology in high dose and control group as well as brains of the medium dose group were processed for histopathology.

**Result:** no decomposition or chamber loss of the metered TS; at the high concentration all females and 10/30 male rats died between the 2nd and 6th week with acute degenerations in the deep cerebellar nuclei, vestibular nuclei and corpora striata and acute lymphoid degenerations in the thymus; 7/15 survivors (non-recovery and recovery group combined) in this group had gliosis and malacia in the same brain regions but no peripheral neuropathy, minimal squamous metaplasia in the nasal mucosa, decreased body and relative organ weights, lymphocytosis, reduced hematocrit and red blood cell counts, increased mean corpuscular hemoglobin and volume, and minor alterations in serum and urine chemistry (last 7 parameters reversible in recovery-group); 5 out of the 7 survivors showed neurobehavioral alterations like abnormal midair righting reflex or impaired gait also at the end of the exposure. At 307 ppm no deaths occurred, but females with slightly decreased body weight gain and in both sexes minor alterations in hematology, serum and urine chemistry (not present in recovery rats). At 101 ppm rats showed no differences from the control rats.

All nonmorphological effects (even minor alteration) significant.

**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** purity=99%

(58)

**Species:** rat **Sex:** no data  
**Strain:** no data  
**Route of admin.:** gavage  
**Exposure period:** 1-15 days, 1-11 applications  
**Frequency of treatment:** once daily  
**Post. obs. period:** no  
**Doses:** 0, 100, 500, 1000 mg/kg  
**Control Group:** yes, concurrent vehicle  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: a) 5 rats per group; at 100 mg/kg 11th dose 1000 mg/kg; b) additional experiments (0 or 100 mg/kg) with 5 male rats per group, 10 applications over 14 d period.  
**Result:** a) 1000 mg/kg (once): rapid onset of dyspnea and depression followed by prostration and death of all rats within 1 h after dosing; no TS related changes at autopsy.  
500 mg/kg: like high dose rats except that tremors and ataxia were observed; 3/5 rats died after 4 applications, 2/5 were sacrificed due to poor condition; autopsy: 2/5 rats with poor haircoats, 1/5 distended bladder, congested lungs, clouding of cornea; histopathology: thymic necrosis (4/5), hepatocytes swelling and hepatic congestion (3/5), nephrosis (1/5), lymphadenitis of mesenteric lymph nodes (3/5), inflammation of the heart (3/5).  
100 mg/kg: slight depression after applications (persisted 24 h in one rat which developed head tilt to the left side); all rats died after the last application or were sacrificed in moribund state; histopathologically no TS related changes.  
b) no differences between the 2 groups with regard to clinical signs, hematology, clinical chemistry, organ weights, gross pathology and histopathology.

**Source:** Wacker - Chemie GmbH Burghausen

(48)

**Species:** rat **Sex:** male  
**Strain:** other  
**Route of admin.:** s.c.  
**Exposure period:** a) 15 or b) 40 weeks  
**Frequency of treatment:** once daily, 5 days per week  
**Post. obs. period:** no  
**Doses:** 200 mg/kg/d  
**Control Group:** yes  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** 6 (a) or 8 (b) Donryu rats per treatment group; 13 control rats (no data about treatment);  
**Result:** a) moderate effects on body weight gain; 4/6 rats showed increased salivation on the 15th day of treatment and disturbances in gait on the 45th day of treatment; thereafter all 6 rats developed spastic paralysis of the hind limbs; significantly reduced motor conduction velocity and sensory conduction velocity (neurophysiological measurement in the rat tail) in the 8-10 week stage of experiment.  
b) no results reported.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** purity>97%

(59)

**Species:** rabbit **Sex:** male  
**Strain:** New Zealand white  
**Route of admin.:** gavage  
**Exposure period:** 1-14 d, 1-10 applications  
**Frequency of treatment:** once daily  
**Post. obs. period:** no  
**Doses:** 0, 250, 500, 1000 mg/kg  
**Control Group:** yes, concurrent vehicle  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: 2 rabbits per group.  
**Result:** 1000 mg/kg: both rabbits died after the 1st dose; congestion of brain, thymus and lungs, hemorrhage in the thymus.  
500 mg/kg: rabbits died on day 9 and 13; both with congestion of the brain, one with hemorrhage in the brain and spinal cord; 1/2 marked thymic atrophy with macrophage infiltration, gastric mucosal hemorrhage and congested lungs.  
250 mg/kg: one rabbit died on day 4 due to bronchopneumonia (aspiration of the TS); the other rabbit showed no TS related changes at termination of the study (14 days).  
**Source:** Wacker - Chemie GmbH Burghausen

(48)

**5.5 Genetic Toxicity 'in Vitro'**

**Type:** Ames test  
**System of testing:** S. typhimurium, TA 92, 98, 100, 104  
**Concentration:** 0.0019-0.048 mM/plate  
**Metabolic activation:** without  
**Result:** positive  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** result: TS inactive towards TA 92, 98, 100; mutagenic effect in TA 104.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** TS distilled before use.

(60)

**Type:** Ames test  
**System of testing:** Salmonella typhimurium TA 98, 100, 104  
**Concentration:**  
**Metabolic activation:** without  
**Result:** positive  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** result: positive in TA 104; specific activity of the TS 2.25 rev./microgramm.  
validity: data from abstract.  
**Source:** Wacker - Chemie GmbH Burghausen

(61)

**Type:** Ames test  
**System of testing:** S. typhimurium TA 98, 100, 1535, 1537, 1538  
**Concentration:** 0.3, 1, 3, 10, 30 mg/plate  
**Metabolic activation:** with and without  
**Result:** negative  
**Method:** other  
**Year:** **GLP:** yes  
**Test substance:** other TS  
**Remark:** method: tested in triplicate; concurrent solvent and positive control.  
results: cytotoxicity at 30 mg/plate.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** purity= 99.2%

(62)

**Type:** Escherichia coli reverse mutation assay  
**System of testing:** WP2uvrA/pKM101  
**Concentration:**  
**Metabolic activation:** with  
**Result:** positive  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: preincubation assay at 37 degree C for 20 min;  
result: specific activity of the test substance 7.73  
rev./microgram.  
valdity: data from abstract.  
**Source:** Wacker - Chemie GmbH Burghausen (61)

**Type:** HGPRT assay  
**System of testing:** CHO cells  
**Concentration:** 0.005-1.5 mg/ml without S9-mix; 0.0005-1.0 mg/ml with S9-mix  
**Metabolic activation:** with and without  
**Result:** negative  
**Method:** other  
**Year:** **GLP:** yes  
**Test substance:** other TS  
**Remark:** method: duplicate cultures; expression period 9-12 days;  
max. concentration selected which did not kill over 90% of  
the cells; 6 concentrations tested; concurrent vehicle and  
positive control.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** purity= 99.2% (63)

**Type:** Sister chromatid exchange assay  
**System of testing:** CHO cells  
**Concentration:** 10-1000 nM/ml medium  
**Metabolic activation:** without  
**Result:** positive  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** result: significant increase in SCE frequency at 500 nM/ml;  
toxicity level ca. 1000 nM/ml.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** TS distilled before use. (60)

**Type:** Sister chromatid exchange assay  
**System of testing:** CHO cells  
**Concentration:** 0.006-0.1 mg/ml without S9-mix; 0.01-0.3 mg/ml with S9-mix  
**Metabolic activation:** with and without  
**Result:** positive  
**Method:** other  
**Year:** **GLP:** yes  
**Test substance:** other TS  
**Remark:** method: 5 h exposure without and 2 h exposure with S9-mix; SCE production determined for the 3 highest doses which did not produce excessive inhibition of cell division; concurrent positive, negative and vehicle control.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** purity= 99.2%

(63)

**Type:** other  
**System of testing:** Bacillus subtilis H17(rec-) and M45(rec+)  
**Concentration:**  
**Metabolic activation:** with  
**Result:** positive  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: liquid Bacillus subtilis/microsome rec-assay; result: negative result without S9 metabolic activation; 50% survival turbidity at 209 mg/l (rec+) and 195 mg/l (rec-) without metabolic activation, 235 and 173 mg/l, respectively with metabolic activation.  
**Source:** Wacker - Chemie GmbH Burghausen

(64)

**Type:** other  
**System of testing:** Salmonella typhimurium TA1535/pSK1002  
**Concentration:** 40 mg/ml  
**Metabolic activation:** with  
**Result:** positive  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** method: the umu-test was used which detects the induction of DNA repair after incubation with genotoxic substances; incubation at 37 degree C for 2-24 h. result: weakly positive results with and without S9 metabolic activation after 2 h incubation; strong positive results with S9 after 24 h incubation; after 4 and 6 h incubation negative results with and without S9.  
**Source:** Wacker - Chemie GmbH Burghausen

(65)

**Type:** other  
**System of testing:** Saccharomyces cerevisiae diploid strain D61.M  
**Concentration:** 0.74, 0.99, 1.48, 1.96% TS in the medium  
**Metabolic activation:** without  
**Result:**  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** other TS  
**Remark:** method: incubation (before plating) with the TS for 2x4 h at 28 degree C, interrupted by 16 or more hours when cells were placed in an ice-bath; evaluation 6-7 d after plating; red colonies in cycloheximide medium reflected point mutation, mitotic recombination or deletion of chromosomal fragments; white colonies reflected aneuploidy (monosomics). validity: no statistical evaluation. result: more red colonies (14.6-22.4) per 10E5 cells than in the positive control (13.4), negative control 6.8; no effects on number of monosomics  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** purity>97%

(66)

**Type:** other  
**System of testing:** CHO cells  
**Concentration:** 0.08, 0.1, 0.12 mg/ml without S9-mix; 0.10, 0.12, 0.14 with S9-mix  
**Metabolic activation:** with and without  
**Result:** positive  
**Method:** other  
**Year:** **GLP:** yes  
**Test substance:** no data  
**Remark:** method: chromosome aberration study; TS concentrations did not produce excessive cytotoxic inhibition of mitotic cells; negative, positive and vehicle control; 2 h treatment period; chromosomes sampled 14 h after the treatment began. results: TS highly clastogenic without metabolic activation (95-100% cells with aberrations) at all 3 dose levels; negative results with metabolic activation.  
**Source:** Wacker - Chemie GmbH Burghausen

(67)

**Type:** other  
**System of testing:** CHO cells  
**Concentration:** 0.01-0.03 mg/ml without and 0.02-0.1 with metabolic activation  
**Metabolic activation:** with and without  
**Result:** positive  
**Method:** other  
**Year:** **GLP:** yes  
**Test substance:** other TS  
**Remark:** method: chromosome aberration study; TS concentrations did not produce excessive cytotoxicity or inhibition of mitotic cells; concurrent negative, positive and vehicle control; 2 h treatment period (cells harvested at 6 or 10 h after start of exposure) with and 6 or 10 h without metabolic activation.  
results: significant increase in aberrations observed at one dose level and at one sample interval in both tests performed with and without metabolic activation.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** purity= 99.2%

(68)

### 5.6 Genetic Toxicity 'in Vivo'

**Type:** Cytogenetic assay  
**Species:** rat **Sex:** male/female  
**Strain:** Sprague-Dawley  
**Route of admin.:** inhalation  
**Exposure period:** 6 hr/day for 5 consecutive days  
**Doses:** 101, 414, 609 and 695 ppm  
**Result:**  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** as prescribed by 1.1 - 1.4  
**Remark:** Method: 14 males and 14 females per group; air control; positive control was cyclophosphamide (30 mg/kg ip). Evaluation at 6 and 24 hr after the final exposure (5/sex/group at each harvest time).  
**Result:** There were no concentration-related increases in the incidences of chromosomal aberrations in male or female rats exposed to 2,4-pentanedione vapor. A single statistically significant increase in aberrations was seen in males of the 101 ppm group (predominantly chromatid breaks), but this was only small and not seen at the 24 hr harvest. Therefore, 2,4-pentanedione was considered not to be clastogenic in this study. Cyclophosphamide gave a positive result.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** The purity was 99 %.

(69)

**Type:** Cytogenetic assay  
**Species:** mouse **Sex:** male/female  
**Strain:** Swiss Webster  
**Route of admin.:** inhalation  
**Exposure period:** 6 hr/day for 5 consecutive days  
**Doses:** 99, 415 and 590 ppm  
**Result:**  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** no data  
**Remark:** Groups of male and female mice were exposed as follows: 10 males and 10 females to air and mid and low concentrations of 2,4-pentanedione, 14 of each sex to the 2,4-pentanedione high concentration, and 5 of each sex to the positive control material (cyclophosphamide, 30mg/kg ip). Evaluation at 6 and 24 hr after the final exposure.  
**Result:** Exposures to 2,4-pentanedione did not produce any statistically significant or exposure concentration related increase in the incidence of micronucleated polychromatophils. Triethylenemelamine produced a positive response.  
**Source:** Wacker - Chemie GmbH Burghausen

(70)

**Type:** Dominant lethal assay  
**Species:** rat **Sex:** male  
**Strain:** Fischer 344  
**Route of admin.:** inhalation  
**Exposure period:** 6 h/day for 5 consecutive days  
**Doses:** 0, 99, 412, 694 ppm, analytical concentration  
**Result:**  
**Method:** other  
**Year:** 1982 **GLP:** yes  
**Test substance:** other TS  
**Remark:** method: study according to EPA guideline "rodent dominant lethal assay" (1982); 20 rats per group;  
**Result:** significant weight loss during exposure at 412 and 694 ppm; no histopathological changes in brain, testis or thymus after 8 weeks of mating; no effect on terminal body and organ weight; no significant effects on reproductive and gestational parameters except increased preimplantation loss at week 4 in the high concentration group.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** purity=99.2%

(71)

**Type:** Micronucleus assay  
**Species:** mouse **Sex:** male/female  
**Strain:** Swiss Webster  
**Route of admin.:** i.p.  
**Exposure period:** single injection  
**Doses:** 200, 400, 650 mg/kg (ca. 25, 50, 80% of experimentally determined LD50)  
**Result:**  
**Method:** other  
**Year:** **GLP:** yes  
**Test substance:** other TS  
**Remark:** method: 5 males and 5 females per group; vehicle control and positive control; evaluation 30, 48, 72 h after dosing;  
**Result:** significant, dose-related increases in the incidence of micronuclei 30 h (two higher doses) and 48 h (all TS treated groups) in male and female mice; active clastogenic agent.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** purity = 99.2%

(72)

**Type:** Micronucleus assay  
**Species:** mouse **Sex:** male/female  
**Strain:** Swiss Webster  
**Route of admin.:** inhalation  
**Exposure period:** 6 h/day for 5 consecutive days  
**Doses:** 97, 405 and 592 ppm  
**Result:**  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** as prescribed by 1.1 - 1.4  
**Remark:** Method: 5 males and 5 females per group; air control; positive control was triethylenemelamine (0.3 mg/kg ip). Evaluation at 24 hr after the final exposure.  
**Result:** Exposures to 2,4-pentanedione did not produce any statistically significant or exposure concentration related increase in the incidence of micronucleated polychromatophils. Triethylenemelamine produced a positive response.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** The purity was 99.9 %, measured by capillary GC.

(73)

**Type:** Micronucleus assay  
**Species:** rat **Sex:** male/female  
**Strain:** Sprague-Dawley  
**Route of admin.:** inhalation  
**Exposure period:** 6 hr/day for 5 consecutive days  
**Doses:** 97, 405 and 592 ppm  
**Result:**  
**Method:** other  
**Year:** **GLP:** no data  
**Test substance:** as prescribed by 1.1 - 1.4  
**Remark:** Method: 5 males and 5 females per group; air control; positive control was triethylenemelamine (0.3 mg/kg ip). Evaluation at 24 hr after the final exposure.  
**Result:** Exposures to 2,4-pentanedione did not produce any statistically significant or exposure concentration related increase in the incidence of micronucleated polychromatophils. Triethylenemelamine produced a positive response.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** The purity was 99.9 %, measured by capillary GC.

(73)

### 5.7 Carcinogenicity

-

### 5.8 Toxicity to Reproduction

-

### 5.9 Developmental Toxicity/Teratogenicity

**Species:** rat **Sex:** female  
**Strain:** Fischer 344  
**Route of admin.:** inhalation  
**Exposure period:** gestational days (GD) 6-15  
**Frequency of treatment:** 6 h/day  
**Duration of test:** GD 21  
**Doses:** 0, 53, 202, 398 ppm, analytically measured  
**Control Group:** yes, concurrent vehicle  
**NOEL Maternalt.:** = 53 ppm  
**NOEL Teratogen.:** = 53 ppm  
**Method:** other  
**Year:** **GLP:** yes  
**Test substance:** other TS  
**Remark:** method: daily analytical measurement of TS concentration; 25 rats per group; the following parameters were determined: number of pregnant and nonpregnant dams at sacrifice, number of fully resorbed litters, maternal body weight gain, maternal relative and absolute organ weights (liver, thymus and uterine), histopathological findings of maternal brains, corpora lutea/dam, implants/litter, preimplantation loss, viable or non-viable implants/litter, live fetuses/litter, sex ratio, fetal body weight, 27 different fetal variations, visceral and skeletal malformations.

**Result:** No decompositional changes or chamber loss of metered TS; maternal tox.: significantly reduced body weight gain at 398 ppm; liver weight significantly increased at 202 ppm; no further significant effects determined; fetal tox.: significant reduction in male and female body weight at 398 ppm and in male fetal b.w. at 202 ppm; one visceral variation (partial fetal atelectasis) significantly increased at 398 ppm; 17 out of 79 observed skeletal variation exhibited significant changes in incidence in the 398 ppm group (for example poorly or unossified phalanges, unossified cervical or poorly ossified thoracic centrum); no differences among the groups in the incidence of external, visceral or skeletal malformations; no further treatment related effects.

**Source:** Wacker - Chemie GmbH Burghausen

**Test substance:** purity=99.2%

(74) (75)

### 5.10 Other Relevant Information

**Type:** Biochemical or cellular interactions

**Remark:** method: rabbit skeletal myofibrils were incubated with the TS to study the alteration of actin in its native state within the myofilament lattice; preparations of native and desensitized myofibrils were incubated with 100 M/M of actin lysine.  
result: actin isolated from TS treated myofibrils contained 0.5 M of enamine/M; in the presence of Ca<sup>2+</sup> Mg<sup>2+</sup>-ATPase activity of TS treated native myofibrils was 110-120% of max. Ca<sup>2+</sup> stimulated activity in untreated controls; authors comment: potentiated "on" state of the myofibrillar ATPase activity by TS treatment.

**Source:** Wacker - Chemie GmbH Burghausen

**Test substance:** no data

(76)

**Type:** Biochemical or cellular interactions

**Remark:** method: acetoacetic decarboxylase was incubated with the substrate acetoacetate and 0, 0.0033, 0.0067, 0.010 mM TS at 30 degree C.  
result: the TS inhibited concentration-dependent the enzyme.

**Source:** Wacker - Chemie GmbH Burghausen

**Test substance:** no data

(77)

**Type:** Biochemical or cellular interactions

**Remark:** method: purified membrane-bound NAD glycohydrolase of rabbit erythrocytes was incubated at pH 7.4 with 2-20 mM of the TS and activity of the enzyme measured for up to 80 min;  
result: TS led to a time-dependent and concentration-dependent inhibition of the enzyme; after 80 min at 20 mM TS the activity was reduced to less than 10% of the initial activity.

**Source:** Wacker - Chemie GmbH Burghausen

**Test substance:** no data

(78)

**Type:** Biochemical or cellular interactions  
**Remark:** method: the human enzyme myeloperoxidase (0.033 units/ml) was incubated in vitro at pH 4.6 with 10 mM TS.  
result: carbon-centered radicals (mutagenicity) were detected using the spin-trapping technique; same results with horseradish peroxidase and chloroperoxidase.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** purity=99% (79)

**Type:** Biochemical or cellular interactions  
**Remark:** method: purified thyroidal NAD+glycohydrolase was treated with 0-400 mM TS at 30 degree C for 30 min.  
result: selective inactivation of the enzyme; activity reduced to ca. 30% at 400 mM to ca. 70% at 100 mM.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** no data (80)

**Type:** Biochemical or cellular interactions  
**Remark:** method: hepatic microsomes from phenobarbital-induced male Wistar rats were incubated for 30 min at 30 degree C with 16 mM TS and a NADPH-generating system; values related to zero-time samples.  
result: binding to the drug metabolizing enzyme cytochrome P-450 ca. 3.0 mM (binding type I, 385-420 nM); NADPH oxidation 1.6 nM/min/mg microsomal protein; cytochrome P-450 loss 12%; 0.21% heme loss; 92% loss of cytochrome b5; 107% loss of NADPH-cyt.-c reductase;  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** no data (81)

**Type:** Biochemical or cellular interactions  
**Remark:** method: the affinities of the TS as organic solvent in biological systems were calculated using solubility parameter technique; the relative energy differences for the TS as solvent and the following biological materials were given: fat at 37 degree C, fat at 23 degree C, water, blood serum, sucrose, urea, Psoriasis scales and lignin.  
result: 0.69, 0.81, 0.96, 1.57, 1.57, 1.31, 0.92, 1.19, respectively.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** no data (82)

**Type:** Biochemical or cellular interactions  
**Remark:** method: murine erythroleukemia cells line 745 MEL were incubated for 5 d with 3-50 mM TS.  
result: the TS was quite toxic in the used concentration range, but the TS was effective in stimulating the induction of hemoglobin production by the cells.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** no data (83)

**Type:** Biochemical or cellular interactions  
**Remark:** method: the respiratory control index of rat mitochondria was determined in Warburg respirometer by incubation with 10 mM TS and 4 different substrates: a) pyruvate, b) succinate, c) alpha-ketoglutarate and d) glutamate. result: significant decrease in a), c) and d).  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** distilled before use. (84)

**Type:** Neurotoxicity  
**Remark:** The TS produced ataxia and disturbances of the gait in rats after repeated treatment for 45 days, despite the motornerve conductive velocity remaining normal (no further information available).  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** no data (85)

**Type:** other  
**Remark:** antimutagenic activity  
method: a) Ames-test; TA 98 bacteria concomitantly exposed to the mutagens 2-naphthohydroxamic acid or 5-20 nM 2-nitrofluorene and 0.01 or 0.02 mM TS for 30 min before plating; b) rat liver yeast transfer RNA exposed to the carcinogen N-acetoxy-2-acetylaminofluorene with 0.1-0.4 mM TS or without the TS for 1 h at 37 degree C. result: a) reduced number of revertants compared to control. b) the TS inhibited concentration dependent the binding of the carcinogen to the transfer RNA.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** no data (86) (87)

### 5.11 Experience with Human Exposure

**Remark:** method: a) absolute odor threshold was the concentration at which 50% of the odor panel observed an odor in the working fountain; b) odor quality. result: a) 0.01 ppm; b) sour/rancid with an unpleasant hedonic tone.  
**Source:** Wacker - Chemie GmbH Burghausen  
**Test substance:** no data (88)

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**7.1 Risk Assessment**

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