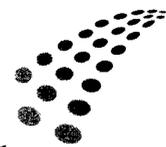


201-14969

**American  
Chemistry  
Council** Good Chemistry  
Makes it Possible



COURTNEY M. PRICE  
VICE PRESIDENT  
CHEMSTAR

December 24, 2003

Michael O. Leavitt, Administrator  
U.S. Environmental Protection Agency  
P.O. Box 1473  
Merrifield, VA 22116  
ATTN: Chemical Right-To-Know Program

RECEIVED  
OPPT/DBIC  
03 DEC 30 PM 3:19

**Re: Benzoyl Chloride Test Plan for Benzoates Panel, HPV Consortium**

Dear Administrator Leavitt:

The American Chemistry Council's Benzoates Panel (Panel) is pleased to submit for review and public comment its Test Plan, including robust summaries, for Benzoyl Chloride (CAS # 98-88-4) under the High Production Volume (HPV) Chemical Challenge Program.

The test plan proposes that the following tests be conducted in order to complete an initial hazard assessment of benzoyl chloride:

- Alga, Growth Inhibition Test (OECD 201)
- Combined Repeated Dose Toxicity with Reproduction/Developmental Toxicity Screening Test (OECD 422)

The Panel understands that there will be a 120-day review period for the test plan and that all comments generated by or provided to EPA will be forwarded to the Panel for consideration.

The Panel members are presently working on an arrangement to fund these tests and, as an alternative, the Panel is considering fulfilling its HPV commitment through the International Council of Chemical Association's (ICCA) HPV Initiative. The Panel will provide EPA with a follow up letter once these decisions are made.



Responsible Care®

Michael O. Leavitt, Administrator  
December 24, 2003  
Page 2 of 2

Please return comments or questions regarding this Test Plan to John Morris, the Panel Manager, at [john\\_morris@americanchemistry.com](mailto:john_morris@americanchemistry.com) or (703) 741-5631.

Sincerely yours,

Courtney M. Price  
Vice President, CHEMSTAR

Attachment

cc with attachment:  
Benzoates Panel  
Steve Russell, ACC  
Jim Keith, ACC

201-14969B

# I U C L I D

## Data Set

RECEIVED  
OPPT 0010  
03 DEC 30 PM 3:20

**Existing Chemical** : ID: 98-88-4  
**CAS No.** : 98-88-4  
**EINECS Name** : benzoyl chloride  
**EC No.** : 202-710-8  
**TSCA Name** : Benzoyl chloride  
**Molecular Formula** : C7H5ClO

**Producer related part**  
**Company** : Bayer Corporation  
**Creation date** : 15.07.1999

**Substance related part**  
**Company** : Bayer Corporation  
**Creation date** : 15.07.1999

**Status** :  
**Memo** : American Chemistry Council, Benzoate HPV Panel

**Printing date** : 16.12.2003  
**Revision date** :  
**Date of last update** : 16.12.2003

**Number of pages** : 40

**Chapter (profile)** : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10  
**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

# 1. General Information

Id 98-88-4  
Date 16.12.2003

## 1.0.1 APPLICANT AND COMPANY INFORMATION

Type : lead organisation  
Name : American Chemistry Council, Benzoate HPV Panel  
Contact person :  
Date :  
Street : 1300 Wilson Boulevard  
Town : 22209 Arlington, VA  
Country : United States  
Phone :  
Telefax :  
Telex :  
Cedex :  
Email :  
Homepage :

05.09.2002

Type : cooperating company  
Name : Atofina Chemicals  
Contact person :  
Date :  
Street :  
Town :  
Country : United States  
Phone :  
Telefax :  
Telex :  
Cedex :  
Email :  
Homepage :

05.09.2002

Type : cooperating company  
Name : Bayer Chemicals Corporation  
Contact person :  
Date :  
Street :  
Town :  
Country : United States  
Phone :  
Telefax :  
Telex :  
Cedex :  
Email :  
Homepage :

05.09.2002

Type : cooperating company  
Name : Velsicol Chemical Corporation  
Contact person :  
Date :  
Street :  
Town :  
Country : United States  
Phone :  
Telefax :

# 1. General Information

Id 98-88-4

Date 16.12.2003

Telex :  
Cedex :  
Email :  
Homepage :

05.09.2002

## 1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

## 1.0.3 IDENTITY OF RECIPIENTS

## 1.0.4 DETAILS ON CATEGORY/TEMPLATE

### 1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name :  
Smiles Code : O=C(c(cccc1)c1)CL  
Molecular formula : C7 H5 Cl1 O1  
Molecular weight : 140.57  
Petrol class :

17.01.2003

### 1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type : typical for marketed substance  
Substance type : organic  
Physical status : liquid  
Purity : > 99.5 % v/v  
Colour :  
Odour :

16.04.2003

### 1.1.2 SPECTRA

## 1.2 SYNONYMS AND TRADENAMES

benzenecarbonyl chloride

16.04.2003

## 1.3 IMPURITIES

## 1.4 ADDITIVES

# 1. General Information

Id 98-88-4

Date 16.12.2003

## 1.5 TOTAL QUANTITY

## 1.6.1 LABELLING

## 1.6.2 CLASSIFICATION

## 1.6.3 PACKAGING

## 1.7 USE PATTERN

### 1.7.1 DETAILED USE PATTERN

### 1.7.2 METHODS OF MANUFACTURE

## 1.8 REGULATORY MEASURES

### 1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

#### Short term exposure limit value

Limit value : .05 other: ppm  
Time schedule :  
Frequency : times

Remark : Ceiling limit  
Critical effect: irritation

06.09.2002

(1)

### 1.8.2 ACCEPTABLE RESIDUES LEVELS

### 1.8.3 WATER POLLUTION

### 1.8.4 MAJOR ACCIDENT HAZARDS

### 1.8.5 AIR POLLUTION

### 1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

### 1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

# 1. General Information

Id 98-88-4  
Date 16.12.2003

## 1.9.2 COMPONENTS

## 1.10 SOURCE OF EXPOSURE

## 1.11 ADDITIONAL REMARKS

## 1.12 LAST LITERATURE SEARCH

## 1.13 REVIEWS

## 2. Physico-Chemical Data

Id 98-88-4

Date 16.12.2003

### 2.1 MELTING POINT

**Value** : = -1 °C  
**Sublimation** :  
**Method** : other: not specified  
**Year** :  
**GLP** : no data  
**Test substance** :  
  
**Reliability** : (2) valid with restrictions  
Data from Handbook or collection of data  
**Flag** : Critical study for SIDS endpoint  
16.12.2003 (2) (3) (4) (5)  
  
**Value** : -6 °C  
Data from Handbook or collection of data  
29.07.1992 (6)

### 2.2 BOILING POINT

**Value** : 197.2 °C at 1013 hPa  
**Decomposition** :  
**Method** : other: Handbook value  
**Year** :  
**GLP** : no data  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted  
  
**Reliability** : (2) valid with restrictions  
Data from Handbook or collection of data  
**Flag** : Critical study for SIDS endpoint  
05.09.2002 (2) (3) (5)  
  
**Value** : 198.3 °C at 1013 hPa  
**Decomposition** :  
**Method** : other: Handbook value  
**Year** :  
**GLP** : no data  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted  
Data from Handbook or collection of data  
05.09.2002 (6)  
  
**Value** : = 198 °C at 1013 hPa  
**Decomposition** :  
**Method** : other: not specified  
**Year** :  
**GLP** : no data  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted  
05.09.2002 (4)  
  
**Value** : 71 °C at 11.99 hPa  
**Decomposition** :  
**Method** : other: Handbook value  
**Year** :  
**GLP** : no data

## 2. Physico-Chemical Data

Id 98-88-4

Date 16.12.2003

**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted  
05.09.2002 (2)

### 2.3 DENSITY

**Type** : density  
**Value** : 1.21 g/cm<sup>3</sup> at 20 °C  
**Method** : other: Handbook value  
**Year** :  
**GLP** : no data  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted  
**Reliability** : (2) valid with restrictions  
Data from Handbook or collection of data  
**Flag** : Critical study for SIDS endpoint  
05.09.2002 (6) (2)

**Type** : density  
**Value** : 1.22 g/cm<sup>3</sup> at 15 °C  
**Method** : other: Handbook value  
**Year** :  
**GLP** : no data  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted  
**Reliability** : (2) valid with restrictions  
Data from Handbook or collection of data  
05.09.2002 (5)

**Type** : density  
**Value** : ca. 1.211 g/cm<sup>3</sup> at 15.5 °C  
**Method** : other: not specified  
**Year** :  
**GLP** : no data  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted  
05.09.2002 (4)

### 2.3.1 GRANULOMETRY

### 2.4 VAPOUR PRESSURE

**Value** : .5 hPa at 20 °C  
**Decomposition** :  
**Method** : other (measured): Handbook value  
**Year** :  
**GLP** : no data  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted  
**Reliability** : (2) valid with restrictions  
Data from Handbook or collection of data  
**Flag** : Critical study for SIDS endpoint  
17.01.2003 (6) (5)

**Value** : = 1.33 hPa at 20 °C  
**Decomposition** :  
**Method** : other (measured): not specified

## 2. Physico-Chemical Data

Id 98-88-4

Date 16.12.2003

<b>Year</b>	:		
<b>GLP</b>	:	no data	
<b>Test substance</b>	:	other TS: benzoyl chloride, CAS# 98-88-4; purity not noted	
05.09.2002			(4)
<b>Value</b>	:	1.1 hPa at 30 °C	
<b>Decomposition</b>	:		
<b>Method</b>	:	other (measured): Handbook value	
<b>Year</b>	:		
<b>GLP</b>	:	no data	
<b>Test substance</b>	:	other TS: benzoyl chloride, CAS# 98-88-4; purity not noted	
05.09.2002			(6)
<b>Value</b>	:	1.33 hPa at 32 °C	
<b>Decomposition</b>	:		
<b>Method</b>	:	other (measured): Handbook value	
<b>Year</b>	:		
<b>GLP</b>	:	no data	
<b>Test substance</b>	:	other TS: benzoyl chloride, CAS# 98-88-4; purity not noted	
<b>Reliability</b>	:	(2) valid with restrictions Data from Handbook or collection of data	
17.01.2003			(3)
<b>Value</b>	:	3.7 hPa at 50 °C	
<b>Decomposition</b>	:		
<b>Method</b>	:	other (measured): Handbook value	
<b>Year</b>	:		
<b>GLP</b>	:	no data	
<b>Test substance</b>	:	other TS: benzoyl chloride, CAS# 98-88-4; purity not noted	
05.09.2002			(6)

### 2.5 PARTITION COEFFICIENT

<b>Partition coefficient</b>	:		
<b>Log pow</b>	:	1.1 at °C	
<b>pH value</b>	:		
<b>Method</b>	:		
<b>Year</b>	:		
<b>GLP</b>	:		
<b>Test substance</b>	:	as prescribed by 1.1 - 1.4	
<b>Remark</b>	:	The partition coefficient for benzoyl chloride was 1.1 using a 1,2-dichlorobenzene/water system.	
<b>Reliability</b>	:	(2) valid with restrictions The study was done using the method of Leo, Hansch and Elkins with one exception - 1,2-dichlorobenzene was used rather than n-octanol because of the formation of esters when benzoyl chloride reacts with n-octanol.	
<b>Flag</b>	:	Critical study for SIDS endpoint	
16.12.2003			(7)
<b>Remark</b>	:	No value due to rapid decomposition in water.	
05.09.2002			(8)

## 2. Physico-Chemical Data

Id 98-88-4

Date 16.12.2003

### 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

**Solubility in** : Water

**Remark** : n.a. (Decomposition)

**Reliability** : (2) valid with restrictions  
Data from Handbook or collection of data

**Flag** : Critical study for SIDS endpoint  
05.09.2002 (5)

**Solubility in** : Water

**pKa** : at 25 °C

**Description** :

**Stable** :

**Remark** : No value due to decomposition in water.  
Decomposition products: - benzoic acid (readily degraded:  
half life = 16 sec.) - Hydrochloric acid

05.09.2002 (4)

### 2.6.2 SURFACE TENSION

### 2.7 FLASH POINT

**Value** : = 68 °C

**Type** : closed cup

**Method** : other: not specified

**Year** :

**GLP** : no data

**Test substance** :

02.03.1998 (4)

**Value** : 93 °C

**Type** : closed cup

**Method** : other: DIN 51755

**Year** :

**GLP** :

**Test substance** :

20.08.1992 (8)

### 2.8 AUTO FLAMMABILITY

**Remark** : ignition temperature: 600 degree C  
13.07.1993 (6)

### 2.9 FLAMMABILITY

### 2.10 EXPLOSIVE PROPERTIES

**Result** : other: explosive limits: lower 2.5 % by vol., upper 27.0 % by vol.

## 2. Physico-Chemical Data

Id 98-88-4

Date 16.12.2003

13.07.1993

(6)

### 2.11 OXIDIZING PROPERTIES

### 2.12 DISSOCIATION CONSTANT

### 2.13 VISCOSITY

### 2.14 ADDITIONAL REMARKS

**Remark**

: Henry's law constant: 1.23E-04 atm-cuM/mole.  
Estimated using HINE, J. and MOOKERJEE, P.K. (1975) bond  
method.  
Decomposition occurs in water.

02.03.1998

(9)

### 3. Environmental Fate and Pathways

Id 98-88-4

Date 16.12.2003

#### 3.1.1 PHOTODEGRADATION

- Remark** : Benzoyl chloride may directly photolyse in the atmosphere.  
The atmospheric half-life for the reaction of benzoyl chloride with photochemically produced hydroxy radicals was estimated to be 2.1 days.
- Reliability** : (2) valid with restrictions  
Data from Handbook or collection of data
- Flag** : Critical study for SIDS endpoint  
16.12.2003 (10)
- Type** : air  
**Light source** :
- Remark** : Benzoyl chloride exhibits an absorption maximum of 282.9 nm and a significant absorption at 293.0 nm in methylcyclohexane.
- | Absorption coefficient | Wavelength (nm) |
|------------------------|-----------------|
| 0.1108E04              | 293.0           |
| 0.1752E04              | 282.9           |
| 0.1390E05              | 249.9           |
| 0.1503E05              | 246.6           |
| 0.1627E05              | 242.0           |
- 06.03.2003 (4) (11)

#### 3.1.2 STABILITY IN WATER

- Type** : abiotic  
**Degradation** : 50 % after 0.3 minute(s) at 2 °C  
**Deg. product** : yes  
**Method** :  
**Year** :  
**GLP** : no data  
**Test substance** :
- Result** : The rate constant for the hydrolysis is  $4 \cdot 10^{-2}$  1/sec at 2 degree C and the hydrolysis half-life is 16 sec.  
The hydrolysis products are benzoic acid and hydrochloric acid.
- Reliability** : (2) valid with restrictions  
Meets generally accepted scientific standards, well documented and acceptable for assessment
- Flag** : Critical study for SIDS endpoint  
17.01.2003 (12) (13) (4)

#### 3.1.3 STABILITY IN SOIL

- Remark** : No data were available, but due to the rapid hydrolysis of benzoyl chloride, the compound is not expected to persist in soil.  
06.09.2002 (4)

### 3. Environmental Fate and Pathways

Id 98-88-4

Date 16.12.2003

#### 3.2.1 MONITORING DATA

#### 3.2.2 FIELD STUDIES

#### 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

**Type** : fugacity model level III  
**Media** : other: air - water - soil - sediment  
**Method** : other: EPIWin Modeling Program  
**Year** :  
**Remark** : Modeling was performed using equal releases (1,000 kg/hr) and equal distribution to all compartments.  
**Result** : Chem Name : Benzoyl chloride  
Molecular Wt: 140.57  
Henry's LC : 0.000132 atm-m<sup>3</sup>/mole (Henrywin program)  
Vapor Press : 0.363 mm Hg (Mpbpwin program)  
Log Kow : 1.44 (Kowwin program)  
**\*\*Acetyl halides hydrolyze....estimate questionable!**  
Soil Koc : 11.3 (calc by model)

	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	14.7	144	1000	1.8e-010
Water	43.3	360	1000	1.44e-009
Soil	41.9	360	1000	2.7e-008
Sediment	0.0891	1.44e+003	0	1.16e-009

	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	498	1.04e+003	16.6	34.6
Water	589	306	19.6	10.2
Soil	570	0	19	0
Sediment	0.303	0.0126	0.0101	0.000419

Persistence Time: 235 hr  
Reaction Time: 426 hr  
Advection Time: 526 hr  
Percent Reacted: 55.2  
Percent Advected: 44.8

**Reliability** : (2) valid with restrictions  
Accepted calculation method  
**Flag** : Critical study for SIDS endpoint

05.09.2002

(14)

**Type** : volatility  
**Media** :  
**Method** :  
**Year** :

**Remark** : No data were available, but due to its rapid hydrolysis, volatilization from the water or soil is not expected to be an important factor of the fate of benzoyl chloride.

06.09.2002

(4)

### 3. Environmental Fate and Pathways

Id 98-88-4

Date 16.12.2003

#### 3.3.2 DISTRIBUTION

#### 3.4 MODE OF DEGRADATION IN ACTUAL USE

#### 3.5 BIODEGRADATION

Type : aerobic  
Inoculum : predominantly domestic sewage  
Concentration : 2.4 mg/l related to related to  
Contact time :  
Degradation : 92 (±) % after 20 day(s)  
Result :  
Kinetic of testsubst. : 5 day(s) 71 %  
10 day(s) 90 %  
20 day(s) 92 %  
Deg. product :  
Method : other: in accordance with the later published OECD Guide-line 301 D  
Year : 1974  
GLP : no  
Test substance : as prescribed by 1.1 - 1.4  
Remark : BOD in proportion to ThOD (theoretical oxygen demand) of 1821 mg O<sub>2</sub>/g substance  
Reliability : (2) valid with restrictions  
Similar to Guideline study  
Flag : Critical study for SIDS endpoint  
17.01.2003 (15)

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

#### 3.7 BIOACCUMULATION

Remark : No value, due to decomposition.  
06.09.2002 (4)

#### 3.8 ADDITIONAL REMARKS

## 4. Ecotoxicity

Id 98-88-4

Date 16.12.2003

### 4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	: static
Species	: Pimephales promelas (Fish, fresh water)
Exposure period	: 96 hour(s)
Unit	: mg/l
LC50	: 34.1
Limit test	:
Analytical monitoring	: yes
Method	:
Year	:
GLP	: no data
Test substance	: other TS: benzoyl chloride, CAS# 98-88-4; purity not noted
Method	: The minnows were raised from controlled breeding stocks at the EPA Newton Fish Toxicology Station, Cincinnati, OH and were observed for a minimum of 14 days prior to testing. The fish were acclimated for 2 days in 100% test dilution water at 22 degree C. Bioassay containers were filled with 12 liters of dilution water. Test substance was added in the form of a stock solution in deionized water. Five fish were placed in each of two duplicate aquaria (10 fish/concentration). At 24 hr intervals, fish were observed for survival, and water tested for dissolved oxygen and temperature. At the end of the 96 hr exposure period, pH and test substance concentration was measured by electron capture gas chromatography (benzene:15% ether extraction). With concentration versus mortality results, 96 hr LC50 and 95% confidence limits were calculated by Probit, Moving average, or Binomial test (depending on the number of partial kills observed).
Remark	: Benzoyl chloride reacted with water to give benzoic acid and HCl, causing a decrease in pH to 5.2 in freshwater and 7.2 in salt water. However, the biological oxygen demand of the benzoic acid was a far more serious effect. In the saltwater test of grass shrimp this was believed to be the major cause of mortality since dissolved oxygen levels plunged below 1 mg/l in direct correspondence to initial benzoyl chloride concentration.
Result	: 95% confidence interval = 28.5 - 45.3 mg/l
Test condition	: Reconstituted soft water of the following quality was used: 40 - 48 mg/l hardness as CaCO3 30 - 35 mg/l alkalinity as CaCO3 120 - 160 uS/cm conductivity pH 7.2 - 7.9 temperature = 22 +/- 1 degree C.
Reliability	: (2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag	: Critical study for SIDS endpoint
06.03.2003	
Type	: static
Species	: Brachydanio rerio (Fish, fresh water)
Exposure period	: 96 hour(s)
Unit	: mg/l
LC0	: 7.5
LC100	: 10
Limit test	:
Analytical monitoring	: no
Method	: other: Letale Wirkung beim Zebrabaerbling, UBA-Verfahrensvorschlag, Mai1984, Letale Wirkung beim Zebrabaerbling Brachydanio rerio LC0, LC50, LC100, 48-96h
Year	: 1987

(16)

## 4. Ecotoxicity

Id 98-88-4

Date 16.12.2003

GLP : no  
Test substance : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted  
  
Method : Lethality Study with the Zebrafish, UBA procedure, May, 1984.  
Result : geometric mean (LC0/LC100) = 8.7 mg/l  
Test condition : ventilated test medium, static system, 10 animals/vessel. The test substance was weighed directly into the dilution water.  
Reliability : (2) valid with restrictions  
Meets National standards method (AFNOR/DIN); no analytical monitoring done  
  
16.12.2003 (17)

Type : static  
Species : Leuciscus idus (Fish, fresh water)  
Exposure period : 72 hour(s)  
Unit : mg/l  
LC0 : 200  
LC100 : 500  
Limit test :  
Analytical monitoring : no  
Method : other: Bestimmung der akuten Wirkung von Stoffen auf Fische, Arbeitskreis "Fischtest" im Hauptausschuss "Detergentien" (15.10.73)  
  
Year : 1974  
GLP : no  
Test substance : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted  
  
Method : Determination of the acute effect of materials on fish (15.10.73).  
Remark : direct weight  
Test condition : 11 test medium, ventilated, static system, 2 animals/vessel.  
Reliability : (2) valid with restrictions  
Test design has some deficiencies. No detailed data given.  
  
06.03.2003 (17)

Type : static  
Species : Pimephales promelas (Fish, fresh water)  
Exposure period : 96 hour(s)  
Unit : mg/l  
LC50 : 34.7  
Limit test :  
Analytical monitoring : yes  
Method :  
Year :  
GLP : no data  
Test substance : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted  
  
Remark : analytical monitoring: GC/ECD  
Result : 24 hour LC50 = 42.6 mg/l (Pimephales promelas)  
48 hour LC50 = 34.7 mg/l (Pimephales promelas)  
Reliability : (2) valid with restrictions  
Meets generally accepted scientific standards  
  
16.12.2003 (18)

### 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static  
Species : Palaemonetes pugio (Crustacea)  
Exposure period : 96 hour(s)  
Unit : mg/l  
LC50 : 180

## 4. Ecotoxicity

Id 98-88-4

Date 16.12.2003

**Analytical monitoring** : yes  
**Method** :  
**Year** :  
**GLP** : no data  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted

**Method** : The grass shrimp were collected from wild populations in an estuary near Galveston Bay, Texas and were observed for a minimum of 10 days prior to testing. Bioassay containers were filled with 12 liters of dilution water. Test substance was added in the form of a stock solution in deionized water. Five grass shrimp were placed in each of two duplicate aquaria (10 fish/concentration). At 24 hr intervals, grass shrimp were observed for survival, and water tested for dissolved oxygen and temperature. At the end of the 96 hr exposure period, pH and test substance concentration was measured by electron capture gas chromatography (benzene:15% ether extraction).  
With concentration versus mortality results, 96 hr LC50 and 95% confidence limits were calculated by Probit, Moving average, or Binomial test (depending on the number of partial kills observed).

**Remark** : Benzoyl chloride reacted with water to give benzoic acid and HCl, causing a decrease in pH to 5.2 in freshwater and 7.2 in salt water. However, the biological oxygen demand of the benzoic acid was a far more serious effect. In the saltwater test of grass shrimp this was believed to be the major cause of mortality since dissolved oxygen levels plunged below 1 mg/l in direct correspondence to initial benzoyl chloride concentration.

**Result** : 95% confidence interval = 139.0 - 233.0 mg/l  
**Test condition** : Synthetic salt water of the following quality was used:  
25 +/- 1 g/l salinity  
30,00 - 40,000 uS/cm conductivity  
pH 8.3 - 8.7  
temperature = 22 +/- 1 degree C.

**Reliability** : (2) valid with restrictions  
Meets generally accepted scientific standards, well documented and acceptable for assessment

**Flag** : Critical study for SIDS endpoint  
17.01.2003 (16) (18)

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

### 4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

**Type** : aquatic  
**Species** : activated sludge  
**Exposure period** : 3 hour(s)  
**Unit** : mg/l  
**EC50** : > 100  
**Analytical monitoring** : no  
**Method** : OECD Guide-line 209 "Activated Sludge, Respiration Inhibition Test"  
**Year** : 1987  
**GLP** : no  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted

**Reliability** : (2) valid with restrictions  
Guideline study  
09.09.2002 (8)

**Type** : aquatic

## 4. Ecotoxicity

Id 98-88-4

Date 16.12.2003

Species : Photobacterium phosphoreum (Bacteria)  
Exposure period : 30 minute(s)  
Unit : mg/l  
EC50 : 12.24  
Analytical monitoring : no  
Method : other: Microtox  
Year :  
GLP :  
Test substance :

09.09.2002

(19)

### 4.5.1 CHRONIC TOXICITY TO FISH

### 4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

### 4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

### 4.6.2 TOXICITY TO TERRESTRIAL PLANTS

### 4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

### 4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

### 4.7 BIOLOGICAL EFFECTS MONITORING

### 4.8 BIOTRANSFORMATION AND KINETICS

### 4.9 ADDITIONAL REMARKS

## 5. Toxicity

Id 98-88-4

Date 16.12.2003

### 5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

#### 5.1.1 ACUTE ORAL TOXICITY

**Type** : LD50  
**Value** : 2528 mg/kg bw  
**Species** : rat  
**Strain** : Wistar  
**Sex** : male  
**Number of animals** : 10  
**Vehicle** : other: none  
**Doses** : 1.0, 1.5, 2.0, 2.5, 3.1, 5.0 ml/kg bw (approx. 1210, 1820, 2420, 3030, 3750, 6040 mg/kg bw)  
**Method** :  
**Year** : 1978  
**GLP** : no  
**Test substance** : as prescribed by 1.1 - 1.4

**Method** : 10 rats/dose, single oral application by gavage, undiluted TS, 6 doses, post application observation time: 14 days, observation for clin. signs, no gross or histopathologic evaluation, statistical method: probit analysis

**Result** : LD 50 = 2.09 ml/kg bw (approx. 2528 mg/kg bw)

Dose [ml/kg bw]	Time of death	//	No of rats		
			death/	/with symptoms/	/used
1.0	-		0	0	10
1.5	3 d		2	10	10
2.0	3 hrs-2 d		5	10	10
2.5	3hrs-3 d		6	10	10
3.1	2 d		9	10	10
5.0	3 hrs-2 d		10	10	10

**Reliability** : signs of intoxication: sedation, extention spasm, reduced general condition (2) valid with restrictions  
Comparable to Guideline study; however no performance of gross and histopathologic evaluation

**Flag** : Critical study for SIDS endpoint

06.03.2003

(20) (21) (4)

**Type** : LD50  
**Value** : ca. 2618 mg/kg bw  
**Species** : rat  
**Strain** : other: Spartan  
**Sex** : male/female  
**Number of animals** : 5  
**Vehicle** : other: corn oil  
**Doses** : 500, 1250, 1984, 3150, 5000, 7940 mg/kg bw  
**Method** : other  
**Year** : 1974  
**GLP** : no  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted

**Method** : Five rats of each sex were used at each dose level except at 7940 mg/kg only 5 males were used. Volumes of 10 ml/kg were used at all dose levels. Rats were observed continuously during the first 4 hours after dosing, at 24 hours, and once daily for 14 days. Body weights were recorded at study initiation and at 14 days.

## 5. Toxicity

Id 98-88-4

Date 16.12.2003

**Result** : All surviving rats exhibited normal body weight gains during the 14 day observation period.

Dose	# males died	# females died
500	0/5	0/5
1250	0/5	0/5
1984	0/5	3/5
3150	1/5	5/5
5000	5/5	5/5
7940	5/5	

LD50 (male rats) = 3619 mg/kg (confidence limits = 3008-4353 mg/kg)

LD50 (female rats) = 1900 mg/kg (confidence limits = 1518-2380 mg/kg)

LD50 (combined) = 2618 mg/kg (confidence limits = 2129-3219 mg/kg)

**Reliability** : (2) valid with restrictions  
Meets generally accepted scientific standards, well documented and acceptable for assessment

06.03.2003

(22)

**Type** : LD50  
**Value** : = 2460 mg/kg bw  
**Species** : rat  
**Strain** :  
**Sex** :  
**Number of animals** :  
**Vehicle** :  
**Doses** :  
**Method** :  
**Year** :  
**GLP** :  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted

06.03.2003

(23)

**Type** : LD50  
**Value** : = 1900 mg/kg bw  
**Species** : rat  
**Strain** :  
**Sex** :  
**Number of animals** :  
**Vehicle** :  
**Doses** :  
**Method** :  
**Year** :  
**GLP** :  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted

06.03.2003

(24)

### 5.1.2 ACUTE INHALATION TOXICITY

**Type** : LC50  
**Value** : ca. 1.45 mg/l  
**Species** : rat  
**Strain** : Wistar  
**Sex** : male  
**Number of animals** : 10  
**Vehicle** : other: air  
**Doses** : 0.190, 0.504, 0.708, 1.453, 1.980 mg benzoyl chloride/l air  
**Exposure time** : 4 hour(s)  
**Method** :

## 5. Toxicity

Id 98-88-4

Date 16.12.2003

**Year** : 1979  
**GLP** : no  
**Test substance** : as prescribed by 1.1 - 1.4

**Method** : 10 males/group exposed to 0.190, 0.504, 0.708, 1.453, 1.980 mg benzoyl chloride/l air, nose-only, for 4 hours at room temperature. Post exposure observation time: 21 days. Necropsy was performed on rats that died during exposure, during observation period and on rats that survived.

**Result** : Mortality: no rats died up to 0.708 mg/l;  
1.453 mg/l: 5/10 rats died within 1 to 19 days,  
1.980 mg/l: 6/10 rats died within 4hrs to 2 days.  
Signs of intoxication were: inactivity, piloerection, unkempt fur, and difficulties in breathing up to 19 days post exposure in all rats.  
Rats that died during the test showed dark red colored lungs always with emphysema, some rats showed lung oedema. Rats that survived showed no pathologic findings up to 0.708 mg/l. At higher concentrations lungs with emphysema and mottled, some showed enlarged adrenals.

**Reliability** : (2) valid with restrictions  
Comparable to Guideline study, however no statistical analysis mentioned.

**Flag** : Critical study for SIDS endpoint  
17.01.2003 (25)

**Type** : LC50  
**Value** : > 2.343 mg/l  
**Species** : rat  
**Strain** : Wistar  
**Sex** : male/female  
**Number of animals** : 20  
**Vehicle** : other: air  
**Doses** :  
**Exposure time** : 1 hour(s)  
**Method** :  
**Year** : 1979  
**GLP** : no  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted

**Method** : 10 males and 10 females exposed to 2343 mg benzoyl chloride/l air, nose-only, for 1 hour at room temperature, post exposure observation time: 21 days, necropsy was performed on rats that died during exposure and during observation period and on rats that survived

**Remark** : mortality: 0/10 (m), 2/10 (f)  
**Result** : Mortality: 0/10 (m), 2/10 (f), time of death after 8-11 days. All rats showed difficulties in breathing, piloerection, inactivity for up to 19 days. Necropsy at the end of the observation time revealed lungs with emphysema and/or mottled.

**Reliability** : (2) valid with restrictions  
Comparable to Guideline study, however exposure to 1 concentration only for only 1 hour.

**Flag** : Critical study for SIDS endpoint  
06.03.2003 (25)

**Type** : LC50  
**Value** : 2 - 200 mg/l  
**Species** : rat  
**Strain** : other: Spartan  
**Sex** : male/female  
**Number of animals** : 10  
**Vehicle** :  
**Doses** : 2.0 and 200 mg/l (aerosol)  
**Exposure time** : 4 hour(s)  
**Method** :  
**Year** :

## 5. Toxicity

Id 98-88-4

Date 16.12.2003

**GLP** : no  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; technical grade, lot # D11-I40-626; purity not noted

**Method** : Groups of 5 male and 5 female rats were placed in a sealed 59 l glass chamber and exposed for 4 hours to a dynamic atmosphere containing mist of the test substance. Addition of test substance was controlled by a Dual Syringe Feeder for 200 mg/l and a Harvard Dual Infusion/Withdrawal pump for 2.0 mg/l. Airflow was regulated with a flowmeter. Rats were observed continually throughout the exposure and for a period of 14 days post-exposure. All rats were necropsied upon death or study termination.

**Result** : 2.0 mg/l:  
1/10 rats died on the 6th day of the observation period. Clinical signs during exposure: increased followed by decreased motor activity; eye squint; salivation; lacrimation; slight and/or marked dyspnea, nasal porphyrin discharge. Clinical signs (day 1 to 7): decreased motor activity, dyspnea, diarrhea.  
From day 8-14 surviving rats appeared normal and exhibited normal body weight gains.  
200mg/l:  
All rats died within 4 hours after initiation of the exposure. Clinical signs during exposure: erythema, gasping dyspnea, and those noted for 2.0 mg/l.

**Reliability** : (2) valid with restrictions  
Meets generally accepted scientific standards, well documented and acceptable for assessment

06.03.2003

(22)

**Type** : LC50  
**Value** : > 1.98 mg/l  
**Species** : rat  
**Strain** : Wistar  
**Sex** : female  
**Number of animals** : 10  
**Vehicle** : other: air  
**Doses** : 0.190, 0.504, 0.708, 1.453, 1.980 mg benzoyl chloride/l air  
**Exposure time** : 4 hour(s)  
**Method** :  
**Year** : 1979  
**GLP** : no  
**Test substance** : as prescribed by 1.1 - 1.4

**Method** : 10 females/conc. exposed to 0.190, 0.504, 0.708, 1.453, 1.980 mg benzoyl chloride/l air, nose-only, for 4 hours at room temperature. Post exposure observation time: 21 days. Necropsy was performed on rats that died during exposure, during observation period and on rats that survived.

**Remark** : Mortality: no rats died up to 0.708 mg/l;  
1.453 mg/l: 1/10 rat died within 10 days,  
1.980 mg/l: 3/10 rats died within 4hrs to 1 day.  
Signs of intoxication were inactivity, piloerection, unkempt fur, and difficulties in breathing up to 19 days post exposure in all rats.  
Rats that died during the test showed dark red colored lungs always with emphysema, some rats showed lung oedema. Rats that survived showed no pathologic findings up to 0.708 mg/l. At higher concentrations lungs with emphysema and mottled, some showed enlarged adrenals.

**Reliability** : (2) valid with restrictions  
No statistical analysis mentioned

06.03.2003

(25)

**Type** : other: IRT  
**Value** : -  
**Species** : rat  
**Strain** : Wistar

## 5. Toxicity

Id 98-88-4

Date 16.12.2003

**Sex** : male/female  
**Number of animals** : 10  
**Vehicle** : other: air  
**Doses** : saturated vapor  
**Exposure time** :  
**Method** :  
**Year** : 1979  
**GLP** : no  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted

**Method** : 5 male and 5 female rats/group; whole-body exposure; exposure time: 1, 3, 7 hours; post exposure observation time: 14 days. Animals observed for clinical signs; necropsy of rats that died during the experiment and of survivors.

**Result** : Mortality: 1hr-, 3hr-exp: no deaths, 7hr-exp.: 2/5 female rats died within 1 to 10 days, 3/5 males died within 2-3 days.  
Signs of intoxication: From 5 min after the start of the exposure up to 14 days post exposure rats showed difficulties in breathing and inactivity (apathy). Irritant effects were observed of the visible mucous membranes of eyes and nose.  
Necropsy of the dead rats: lungs were dark red, emphysema, mottled.  
Necropsy of survivors: signs of developing emphysema of the lungs.

**Reliability** : (2) valid with restrictions  
Comparable to Guideline study, however no information on the concentration of the test atmosphere

06.03.2003

(25)

**Type** : LC50  
**Value** : = 1.87 mg/l  
**Species** : rat  
**Strain** :  
**Sex** :  
**Number of animals** :  
**Vehicle** :  
**Doses** :  
**Exposure time** : 2 hour(s)  
**Method** :  
**Year** :  
**GLP** :  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted

06.03.2003

(24)

### 5.1.3 ACUTE DERMAL TOXICITY

**Type** : LD50  
**Value** : > 2000 mg/kg bw  
**Species** : rabbit  
**Strain** : New Zealand white  
**Sex** : male/female  
**Number of animals** : 4  
**Vehicle** : other: neat  
**Doses** : 2000 mg/kg  
**Method** : other  
**Year** : 1974  
**GLP** : no  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; technical grade, lot # D11-I40-626; purity not noted

## 5. Toxicity

Id 98-88-4

Date 16.12.2003

**Method** : The hair was clipped from the backs of 2 male and 2 female rabbits; the skin of 1 male and 1 female was abraded. The test compound was applied only once to the back of each animal at a dose of 2000 mg/kg. The area was wrapped with gauze and plastic wrap. 24 hours later, the bandages were removed and the backs washed with tepid water. The rabbits were observed for toxicity and mortality for a period of 14 days.

**Remark** : None of the rabbits died during treatment and during the observation period. 3/4 rabbits exhibited normal body weight gains. All rabbits exhibited fissuring on the site of application.

**Reliability** : (2) valid with restrictions  
Meets generally accepted scientific standards, well documented and acceptable for assessment

**Flag** : Critical study for SIDS endpoint  
06.03.2003 (22)

**Type** : LD50  
**Value** : = 790 mg/kg bw  
**Species** : rabbit  
**Strain** :  
**Sex** :  
**Number of animals** :  
**Vehicle** :  
**Doses** :  
**Method** :  
**Year** :  
**GLP** :  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted  
06.03.2003 (23)

### 5.1.4 ACUTE TOXICITY, OTHER ROUTES

### 5.2.1 SKIN IRRITATION

**Species** : rabbit  
**Concentration** : undiluted  
**Exposure** : Semiocclusive  
**Exposure time** : 4 hour(s)  
**Number of animals** : 6  
**Vehicle** :  
**PDII** : 3.8  
**Result** : irritating  
**Classification** :  
**Method** : other: similar to Draize test  
**Year** : 1974  
**GLP** : no  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; technical grade, lot # D11-I40-626; purity not noted

**Method** : The hair was clipped from the backs of 3 male and 3 female New Zealand White rabbits; the skin of 3 animals was abraded. 0.5 ml of test material was applied to the back of each animal and the area wrapped with a gauze bandage. Four hours later the bandage was removed and the area washed with tepid water. The skin was evaluated for irritation immediately and at 24 and 72 hours.

**Remark** : primary irritation scor: 3.8  
**Reliability** : (2) valid with restrictions  
Meets generally accepted scientific standards, well documented and

## 5. Toxicity

Id 98-88-4

Date 16.12.2003

Flag : acceptable for assessment  
06.03.2003 : Critical study for SIDS endpoint (22)

Species : rabbit  
Concentration : undiluted  
Exposure : Occlusive  
Exposure time : 24 hour(s)  
Number of animals : 2  
Vehicle :  
PDII :  
Result : corrosive  
Classification :  
Method : other: see remarks  
Year : 1979  
GLP : no  
Test substance : as prescribed by 1.1 - 1.4

Method : 2 rabbits, 0.5 ml/animal applied on a gauze patch which was fixed with a plaster to the ear for 24 hrs, post exposure observation time: 7 d, no information about evaluation method.

Result : After removal of the plaster: severe erythema and edema up to 7 days (no scores available) and within the last observation days: necrosis.

Reliability : (2) valid with restrictions  
Deficiencies in the description of test performance.  
06.03.2003 (25)

### 5.2.2 EYE IRRITATION

Species : rabbit  
Concentration : undiluted  
Dose : .1 ml  
Exposure time : 5 minute(s)  
Comment : rinsed after (see exposure time)  
Number of animals : 5  
Vehicle :  
Result : corrosive  
Classification :  
Method : other: similar to Draize  
Year :  
GLP : no  
Test substance : other TS: benzoyl chloride, CAS# 98-88-4; technical grade, lot # D11-I40-626; purity not noted

Method : 5 rabbits; 0.1 ml/animal was placed into the conjunctival sac of right eye of each rabbit, left eye served as untreated control. Post exposure observation: 1, 24, 48, 72 hours, 7, 14, and 21 days. Evaluation was done with sodium fluorescein.

Reliability : (2) valid with restrictions  
Meets generally accepted scientific standards, well documented and acceptable for assessment

Flag : Critical study for SIDS endpoint  
06.03.2003 (22)

Species : rabbit  
Concentration : undiluted  
Dose : .1 ml  
Exposure time : 24 hour(s)  
Comment : rinsed after (see exposure time)  
Number of animals : 3

## 5. Toxicity

Id 98-88-4

Date 16.12.2003

**Vehicle** :  
**Result** : corrosive  
**Classification** :  
**Method** : other: similar to Draize  
**Year** : 1974  
**GLP** : no  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; technical grade, lot # D11-I40-626; purity not noted

**Method** : 5 rabbits; 0.1 ml/animal was placed into the conjunctival sac of right eye of each rabbit, left eye served as untreated control. Post exposure observation: 1, 24, 48, 72 hours, 7, 14, and 21 days. Evaluation was done with sodium fluorescein.

**Reliability** : (2) valid with restrictions  
Meets generally accepted scientific standards, well documented and acceptable for assessment

06.03.2003

(22)

**Species** : rabbit  
**Concentration** : undiluted  
**Dose** : .1 ml  
**Exposure time** :  
**Comment** :  
**Number of animals** : 2  
**Vehicle** :  
**Result** : corrosive  
**Classification** :  
**Method** :  
**Year** : 1979  
**GLP** : no  
**Test substance** : as prescribed by 1.1 - 1.4

**Method** : 2 rabbits; 100 ul/animal was placed into the conjunctival sac of one eye of each rabbit, post exposure observation time: 7 days. Evaluation method not described.

**Result** : Conjunctiva: severe redness, moderate to severe chemosis up to the end of the observation period;  
Iris: slight to moderate swollen and hyperemic;  
slight diffuse cornea opacity.

**Reliability** : (2) valid with restrictions  
Deficiencies in the description of test performance.

06.03.2003

(25)

### 5.3 SENSITIZATION

### 5.4 REPEATED DOSE TOXICITY

**Type** : Sub-chronic  
**Species** : mouse  
**Sex** :  
**Strain** :  
**Route of admin.** : inhalation  
**Exposure period** : 5 months  
**Frequency of treatm.** : 30min/d; 2d/w  
**Post exposure period** :  
**Doses** :  
**Control group** :  
**Method** :

## 5. Toxicity

Id 98-88-4

Date 16.12.2003

**Year** :  
**GLP** : no data  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted

**Result** : Mice exposed to benzoyl chloride vapor developed pulmonary tumors (3/28) and skin tumors (2/28). However these results were not significantly different from controls.

**Reliability** : (3) invalid  
Documentation insufficient for assessment

16.12.2003 (26)

**Type** : Sub-chronic  
**Species** : mouse  
**Sex** : female  
**Strain** : other: Specific-Pathogen-Free (SPF) ICR  
**Route of admin.** : dermal  
**Exposure period** : 41 w; 50 w  
**Frequency of treatm.** : 3/w 4 w, 2/w 37 w; 2/w 50 w  
**Post exposure period** : 51- 80 w  
**Doses** : 5 ul, 10 ul; 2.3 ul /animal/painting  
**Control group** : yes  
**Method** :  
**Year** :  
**GLP** : no data  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted

**Result** : For a few minutes after application: marked irritation of the eyes, the skin, and the respiratory system, elevated motor activities; at the painted area: erythema, swelling, later alopecia, induration, marked keratinization, ulcers and/or necrosis of the epidermis.

**Reliability** : (3) invalid  
Documentation insufficient for assessment

16.12.2003 (27) (28)

**Type** :  
**Species** : mouse  
**Sex** : no data  
**Strain** : other: C57 black  
**Route of admin.** : other: intradermal injection  
**Exposure period** : 4 d  
**Frequency of treatm.** : daily  
**Post exposure period** : 24 w  
**Doses** : 5 mg/animal  
**Control group** : no data specified

**Result** : no depigmentation

09.09.2002 (29)

### 5.5 GENETIC TOXICITY 'IN VITRO'

**Type** : Ames test  
**System of testing** : Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537  
**Test concentration** : (1) 0,15, 30, 60, 120, 240, 480 ug/tube; (2) 0, 75, 150, 300, 600, 1200 ug/tube; (3) 225, 450, 900, 1800, 3600 ug/tube; (4) 0, 225, 450, 900, 1800, 3600 ug/tube  
**Cytotoxic concentr.** : from 1200 ug/tube; substance precipitation at 450 ug/tube and above  
**Metabolic activation** : with and without  
**Result** : negative  
**Method** : other: in agreement with OECD 471, preincubation method, solvent: acetone

## 5. Toxicity

Id 98-88-4

Date 16.12.2003

**Year** : 1988  
**GLP** : yes  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted

**Reliability** : (1) valid without restriction  
GLP Guideline study

**Flag** : Critical study for SIDS endpoint  
06.03.2003 (30)

**Type** : Ames test  
**System of testing** : Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538, D4  
**Test concentration** : 0.0001 - 1 ul/plate  
**Cycotoxic concentr.** : 1 ul/plate  
**Metabolic activation** : with and without  
**Result** : negative  
**Method** : other: similar to OECD Guide-line 471  
**Year** :  
**GLP** : no  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted

**Remark** : S9 activation homogenate was prepared from Aroclor 1254-induced Sprague-Dawley adult male rat liver.  
Negative control: DMSO (50 ul/plate).  
Positive controls (non-activated):  
TA-1535, TA-100: ethylmethane sulfonate (10 ul/plate)  
TA-1537: quinacrine mustard (10 ug/plate)  
TA-1538, TA-98: 2-nitrofluorine (10 ug/plate)  
Positive controls (activated):  
all strains: 2-anthramine (2.5 ug/plate)

**Reliability** : (2) valid with restrictions  
Comparable to Guideline study

**Flag** : Critical study for SIDS endpoint  
06.03.2003 (31)

**Type** : Ames test  
**System of testing** : Salmonella typhimurium TA 98, TA 100  
**Test concentration** : 0.1, 1, 10 umole/plate  
**Cycotoxic concentr.** :  
**Metabolic activation** : without  
**Result** : ambiguous  
**Method** : EPA OTS 798.5265  
**Year** :  
**GLP** : no  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted; purchased from Eastman Organic Chemicals, Rochester, NY, USA

**Result** : Benzoyl chloride was mutagenic for TA98 only.  
06.02.2003 (32)

**Type** : Escherichia coli reverse mutation assay  
**System of testing** : Escherichia coli H/r30R, Hs30R  
**Test concentration** :  
**Cycotoxic concentr.** :  
**Metabolic activation** : no data  
**Result** : negative  
**Method** :  
**Year** :  
**GLP** :  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted  
09.09.2002 (33)

## 5. Toxicity

Id 98-88-4

Date 16.12.2003

**Type** : Ames test  
**System of testing** : Salmonella typhimurum G46, TA1535, TA100, C3076, TA1537, D3052, TA1535,TA98  
**Test concentration** :  
**Cycotoxic concentr.** :  
**Metabolic activation** : with and without  
**Result** : negative  
**Method** :  
**Year** :  
**GLP** : no  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted

**Remark** : Gradient plate technique was used which results in a range of concentrations over which chemically-induced mutant colonies are present.  
06.02.2003 (34)

**Type** : Escherichia coli reverse mutation assay  
**System of testing** : E. coli WP2, WP2 uvrA-  
**Test concentration** :  
**Cycotoxic concentr.** :  
**Metabolic activation** : with and without  
**Result** : negative  
**Method** :  
**Year** :  
**GLP** : no  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted

**Remark** : Gradient plate technique was used which results in a range of concentrations over which chemically-induced mutant colonies are present.  
06.02.2003 (34)

**Type** : Escherichia coli reverse mutation assay  
**System of testing** : E. coli WP2 B/r try, WP2 try hcr  
**Test concentration** :  
**Cycotoxic concentr.** :  
**Metabolic activation** : with and without  
**Result** : negative  
**Method** :  
**Year** :  
**GLP** : no  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted; purchased from Tokyo Kasei Co. Ltd.

06.02.2003 (35)

**Type** : Ames test  
**System of testing** : Salmonella typhimurium TA98, TA100, TA104  
**Test concentration** : up to 1000 ug/plate  
**Cycotoxic concentr.** :  
**Metabolic activation** : with and without  
**Result** : positive  
**Method** : other: preincubation method  
**Year** : 1996  
**GLP** : no data  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted

09.09.2002 (36)

**Type** : Bacterial gene mutation assay  
**System of testing** : Escherichia coli WP2uvrA/pKM101  
**Test concentration** : up to 1000 ug/plate  
**Cycotoxic concentr.** :

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**Metabolic activation** : with and without  
**Result** : positive  
**Method** : other: preincubation method  
**Year** : 1996  
**GLP** : no data  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted

09.09.2002 (36)

**Type** : Bacillus subtilis recombination assay  
**System of testing** : B. subtilis H17 (Rec+), M45 (Rec-)  
**Test concentration** :  
**Cycotoxic concentr.** :  
**Metabolic activation** : with and without  
**Result** : negative  
**Method** :  
**Year** :  
**GLP** : no  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted; purchased from Tokyo Kasei Co. Ltd.

06.02.2003 (35)

### 5.6 GENETIC TOXICITY 'IN VIVO'

**Type** : Micronucleus assay  
**Species** : mouse  
**Sex** : male/female  
**Strain** :  
**Route of admin.** : gavage  
**Exposure period** : once  
**Doses** : 0, 1750 mg/kg bw dissolved in corn oil  
**Result** : negative  
**Method** : OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"  
**Year** :  
**GLP** : yes  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity = 99.97 %

**Result** : There were no indications of a clastogenic effect on the chromosomes of the bone marrow erythroblasts.

**Reliability** : (1) valid without restriction  
GLP Guideline study

**Flag** : Critical study for SIDS endpoint

17.01.2003 (37)

### 5.7 CARCINOGENICITY

**Species** : mouse  
**Sex** : female  
**Strain** : other: Specific-Pathogen-Free (SPF) ICR  
**Route of admin.** : dermal  
**Exposure period** : 43 w  
**Frequency of treatm.** : 3/w 4 w, 2/w 39 w  
**Post exposure period** : no  
**Doses** : 5 ul (in 5 ul benzene), 10 ul /animal/painting  
**Result** : negative  
**Control group** : yes  
**Method** :

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**Year** :  
**GLP** :  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted  
**Method** : Two skin painting studies were performed: 10 ul (12.1mg) was applied for 47 weeks  
**Result** : 5 ul-group: 10 animals, 143 d after first application first skin papilloma; 10 ul-group: 10 animals; 2/10 (5 ul), 3/10 (10 ul) with tumors: skin-papilloma and -carcinoma, lung-adenoma. These tumor incidences are not statistically significant as treatment-related carcinogenic effects.

06.03.2003

(27) (28)

**Species** : mouse  
**Sex** : female  
**Strain** : other: Specific-Pathogen-Free (SPF) ICR  
**Route of admin.** : dermal  
**Exposure period** : 50 w  
**Frequency of treatm.** : 2/w  
**Post exposure period** : 51 - 80. w  
**Doses** : 2.3 ul/animal/painting in benzene  
**Result** : negative  
**Control group** : yes  
**Method** :  
**Year** :  
**GLP** :  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; commercial grade, obtained from Wako Pure Chemical Industries Co. Ltd., Tokyo

**Method** : The backs of the mice were clipped free of hair. Benzene was used as the vehicle control. and applied In one experiment, 10 ul (neat) or 5 ul (1:1 with benzene) was administered to the dorsal skin of 3-week old weanling mice with a micropipette 3 times/week for 4 weeks, then twice a week for 9.8 months. Mice were necropsied at 9.8 months. In the second experiment, 2.3 ul (diluted to 25ul with benzene) was administered to 7-week old mice 2 times/week for 50 weeks (11.7 months). At 18.7 months, mice were sacrificed and completely necropsied. After gross examination, organs and tissues were prepared for histological examination.

**Result** : 20 animals, 364 days after first application of 2,3 ul to first skin papilloma (143 days with 5 ul); in the low dose group : 2/20 skin-carcinomas; 5/20 lung-adenomas; mortality at the termination of the experiment = 5 %. These tumor incidences are not statistically significant as treatment-related carcinogenic effects.

Dose	# animals	# skin tumors	# lung tumors
Control	30	0	2
10 ul	10	0	3
5 ul	10	1	0
2.3 ul	20	2	5

06.02.2003

(27) (28)

**Species** : mouse  
**Sex** : no data  
**Strain** : no data  
**Route of admin.** : inhalation  
**Exposure period** : 20 w  
**Frequency of treatm.** : 30 min/d, 2 d/w, 5 months  
**Post exposure period** : several months  
**Doses** : saturated vapor  
**Result** : negative  
**Control group** : yes

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**Method** :  
**Year** :  
**GLP** : no data  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted

**Method** : Mice were exposed to benzoyl chloride vaporized at 50 degree Celsius for 30 minutes/day, 2 days/week for 5 months. Each animal was then observed for several months without subsequent exposures.

**Remark** : article in Japanese with English abstract  
**Result** : Compared to the control, no significant increase in the incidence of pulmonary tumors and skin tumors.

**Reliability** : (4) not assignable  
Original reference in foreign language; Abstract in English

20.11.2003 (26)

**Species** : mouse  
**Sex** : female  
**Strain** : other: ICR-JCL  
**Route of admin.** : inhalation  
**Exposure period** : 20 w  
**Frequency of treatm.** : 30 min, 2/w  
**Post exposure period** : 56 w  
**Doses** : 1.6 ppm  
**Result** :  
**Control group** : no data specified  
**Method** :  
**Year** :  
**GLP** :  
**Test substance** : other TS: benzoyl chloride, CAS# 98-88-4; purity not noted

**Result** : after 24 w: no lesions or tumors; after 40 w: 2 skin papillomas, epithelial proliferation of the trachea; after 56 w: lung adenocarcinomas, lung adenoma

09.09.2002 (38)

**Species** : mouse  
**Sex** : female  
**Strain** : ICR  
**Route of admin.** : inhalation  
**Exposure period** : 20 w  
**Frequency of treatm.** : 30 min, 2/w  
**Post exposure period** : 20 w  
**Doses** : 6.8 ppm  
**Result** :  
**Control group** : no data specified  
**Method** :  
**Year** :  
**GLP** :  
**Test substance** :

**Result** : no lung cancer; trachea and intra-pulmonary bronchi: mild adenoid proliferation

09.09.2002 (39)

### 5.8.1 TOXICITY TO FERTILITY

06.09.2002

## 5. Toxicity

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06.03.2003

### 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

### 5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

## 5.9 SPECIFIC INVESTIGATIONS

## 5.10 EXPOSURE EXPERIENCE

**Type of experience** : Direct observation, clinical cases

**Remark** : Case-report: male, born 1929, engaged in manufacturing of benzoyl chloride from 1955-1969, since 1965 he suffered from frequent colds, bronchial pain, and anosmia. 1969 the skin of his hands coloured black with white and red spots and warts. Since 1971 daily coughing. 1973 diagnosis of a squamous cell carcinoma in the left hilum of the lung.

06.02.2003

(40)

**Type of experience** : Direct observation, clinical cases

**Remark** : Case-report: male, born 1926, engaged in manufacturing of benzoyl chloride from 1954-1969. Since 1970 he suffered from pain in the right chest and coughing, diagnosis by x-ray examination: lung cancer, death in 1972.

06.02.2003

(40)

**Type of experience** : Direct observation, clinical cases

**Remark** : Case-report: male, born 1916, working in an chemical plant somewhere until 1953, engaged in manufacturing of benzoyl chloride from 1954-1960. 1960 diagnosis by x-ray examination: lung cancer, death in 1963.

06.02.2003

(40)

**Type of experience** : Direct observation, clinical cases

**Remark** : Case-report: male, born 1923, engaged in manufacturing of benzoyl chloride from 1960-1970. Since 1970 he suffered from hemorrhagic rhinorrhoe. 1972 diagnosis: maxillary malignant lymphoma, death in 1973.

06.02.2003

(40)

**Type of experience** : Human - Epidemiology

**Remark** : A mortality study of workers in a factory producing chlorinated toluenes showed an increased risk of cancer mortality in workers who had first been employed prior to 1951.

06.02.2003

(41)

**Type of experience** : Human - Epidemiology

**Remark** : The results of a cohort study among workers in a factory manufacturing chlorinated toluenes (follow up period: 1964-1984) showed an excess mortality from lung cancer

06.02.2003

(42)

## 5. Toxicity

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- Type of experience** : Human - Epidemiology
- Remark** : The results of a cohort mortality study of employees exposed to chlorinated toluenes showed a statistically significant increase in lung cancer mortality among employees with 15 or more years of employment.
- 06.02.2003 (43)
- Type of experience** : Direct observation, clinical cases
- Remark** : Case report: male, born in 1929, 1952-1969 engaged in manufacture of benzoyl peroxide, 1956-1963 engaged in the manufacture of benzoyl chloride as overtime work. 1969: suffering from a severe cold, x-ray examination: lung cancer, death: 1970. Necropsy: primary lung cancer with metastases in the pancreas, the kidneys and the back peritoneum.
- 06.02.2003 (44)
- Type of experience** : Direct observation, clinical cases
- Remark** : case report: male, born in 1937, 1957-1961 working in benzoyl peroxide manufacturing process, 1960-1961 working in benzoyl chloride producing process as overtime work and 1961-1962 as regular work, 1962-1969 in the office, since 1962 suffering from a severe cough and dyspnoe, diagnosis: obstructive lung disease, 1972 x-ray examination: lung cancer, death in 1973
- 06.02.2003 (44)
- Type of experience** : Human - Epidemiology
- Remark** : An epidemiolgy study of all workers in a specific chemical plant calculated the expected number of lung cancer deaths as 0.22, but 2 were observed. Among benzoyl chloride workers specifically, the expected number of lung cancer deaths was 0.16, but the observed deaths were 2.
- 06.02.2003 (45)

### 5.11 ADDITIONAL REMARKS

- Type** : Toxicokinetics
- Remark** : A single oral dose of labelled benzoyl chloride (9-13 mg/kg bw) administered to rats was rapidly absorbed from gastrointestinal tract. Elimination: 90 % via urine and 2 % via feces within 48 hrs. Radiocarbon in the blood peaked at about 4 ppm by 1 hr after dosing and then dropped rapidly to 0.02 ppm by 24 hrs. Total radiocarbon in all tissues were found to be low with 0.12 % present after 48 hrs. The half-life of labelled benzoyl chloride in the blood was 1.5 hrs. Over 90 % of the metabolites in the urine were identified as benzoic acid and hippuric acid.
- 06.09.2002 (31)
- Type** : other
- Remark** : Single inhalation: 10 rats/group, 2.0, 200 mg/L, 4 hrs, 14 days observation period.  
200 mg/l: all rats died within the 4 hr-exposure period.  
2 mg/l: mortality: 1/10; signs during exposure and up to d 7: increased motor activity followed by decreased motor activity, eye squint, salivation, lacrimation, both slight and marked dyspnea, nasal porphyrin discharge; from d 8 until the end of the study period the rats appeared normal.

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06.09.2002		(31)
<b>Type</b>	: other	
<b>Remark</b>	: Benzoyl chloride did not show any effect on the metabolic cooperation in Chinese hamster V79 cells at non-cytotoxic concentrations.	
06.09.2002		(46)
<b>Remark</b>	: Benzoyl chloride was identified as inducer of lipid peroxidation in liver, kidney, and spleen tissue in vitro.	
06.09.2002		(47)
<b>Remark</b>	: Pretreatment of E.coli H/r30R with benzoyl chloride showed no effect on UV-induced mutagenesis	
29.07.1992		(33)
<b>Remark</b>	: single inhalation: 5 rats/sex/group, Wistar TNO/W 74, m and f, saturated vapor, 1 h: no deaths; 3 h: no deaths; 7 h: mortality: 2/5 (m), 3/5 (f); all groups: respiratory disease, irritation of the visible mucous membranes of the eyes and the nose	
29.07.1992		(48)
<b>Remark</b>	: Benzoyl chloride has no effect on wound healing when applied into an incision made on the dorsal skin tissue of male Wistar rats.	
06.09.2002		(49)
<b>Remark</b>	: Only a small amount of radioactivity was found in the urine and the feces after application of 10 ul labelled benzoyl chloride through a small incision on the dorsal musculature of male Wistar rats, measured over a period of 15 d. Organ distribution of radioactivity 3 d after application of 10 ul labelled benzoyl chloride through a small incision on the dorsal musculature of male Wistar rats: brain < heart < kidneys < lungs < spleen < skin/muscle	
06.07.1993		(49)

## 6. Analyt. Meth. for Detection and Identification

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### 6.1 ANALYTICAL METHODS

### 6.2 DETECTION AND IDENTIFICATION

## 7. Eff. Against Target Org. and Intended Uses

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7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

## **8. Meas. Nec. to Prot. Man, Animals, Environment**

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**8.1 METHODS HANDLING AND STORING**

**8.2 FIRE GUIDANCE**

**8.3 EMERGENCY MEASURES**

**8.4 POSSIB. OF RENDERING SUBST. HARMLESS**

**8.5 WASTE MANAGEMENT**

**8.6 SIDE-EFFECTS DETECTION**

**8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER**

**8.8 REACTIVITY TOWARDS CONTAINER MATERIAL**

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## 10. Summary and Evaluation

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### 10.1 END POINT SUMMARY

### 10.2 HAZARD SUMMARY

### 10.3 RISK ASSESSMENT