

## REACH Praxisführer zur Expositionsbewertung und zur Kommunikation in den Lieferketten

### Beispiele zu Teil II: Expositionsszenarien und Kommunikation in den Lieferketten

#### **Beispiel 2: Stoffsicherheitsbericht Kaliumtertiärbutylat**

Dieses Beispiel veranschaulicht die Stoffsicherheitsbeurteilung eines Stoffes, zu dem nur begrenzte Daten öffentlich verfügbar sind.

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Das vorliegende Dokument gehört zum Teil II des „REACH Praxisführers zur Expositionsbewertung und zur Kommunikation in den Lieferketten“. Der Praxisführer besteht aus mehreren Teilen. Eine Übersicht finden Sie im Vorwort zu Teil I.

Eine Beschreibung der Inhalte und des Praxisführers steht auf der folgenden Internetseite zur Verfügung:

VCI: <http://www.vci.de/default~cmd~shd~docnr~125022~lastDokNr~102474.htm>

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CEFIC: <http://cefic.org/templates/shwPublications.asp?HID=750>

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**Note**

This Chemical Safety Report is an **example** CSR prepared for the Verband der Chemischen Industrie (VCI) CSA/CSR/eSDS Project. Publicly available data was used to prepare this example CSR. Data was obtained from available IUCLID datasets, downloadable from the European Chemicals Bureau's website. The editor is aware that used data may be owned by other parties. However, the editor considers the question of data ownership not relevant, as this example CSR is prepared for educational purposes only, not for commercial or regulatory purposes.

For the purpose of the mentioned project several simplifications to real life data/situations were adopted (e.g. only two uses were assessed), with the aim to focus on the educational value of the mentioned project. This document should only be used for the purpose of the VCI CSA/CSR/eSDS project and resulting publications.

**CHEMICAL SAFETY REPORT**

<b>Substance Name:</b>	<b>Potassium tert-butate</b>
<b>EC Number:</b>	<b>212-740-3</b>
<b>CAS Number:</b>	<b>865-47-4</b>
<b>Editor:</b>	<b>Dr. Christoph Müller</b> <b>Merck KGaA, Darmstadt, Germany</b>

## CONTENTS

<b>PART A</b>	7
1 SUMMARY OF RISK MANAGEMENT MEASURES	7
2 DECLARATION THAT RISK MANAGEMENT MEASURES ARE IMPLEMENTED	7
3 DECLARATION THAT RISK MANAGEMENT MEASURES ARE COMMUNICATED	7
<b>PART B</b>	8
1 IDENTITY OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES	8
1.1 Name and other identifiers of the substance	8
1.2 Composition of the substance	8
1.3 Physico-chemical properties	9
2 MANUFACTURE AND USES	10
2.1 Manufacture	10
2.2 Identified uses	10
Use 0: Production of potassium tert-butyrate	11
2.3 Uses advised against	11
3 CLASSIFICATION AND LABELLING (ANNEX I OF DIRECTIVE 67/548/EEC)	12
3.1 Potassium tert-butyrate	12
3.1.1 Self classification(s)	12
3.2 Tert-butyl alcohol	12
3.3 Potassium Hydroxide	12
4 ENVIRONMENTAL FATE PROPERTIES	13
4.1 Degradation	13
4.1.1 Abiotic degradation	13
4.1.1.1 Hydrolysis	13
4.1.1.2 Phototransformation/photolysis	13
4.1.1.2.1 Phototransformation in air	13
4.1.1.2.2 Phototransformation in water	13
4.1.1.2.3 Phototransformation in soil	13
4.1.2 Biodegradation	13
4.1.2.1 Biodegradation in water	14
4.1.2.1.1 Screening tests	14
4.1.2.2 Biodegradation in sediments	14
4.1.2.3 Biodegradation in soil	14
4.1.2.4 Summary and discussion on biodegradation	14
4.1.3 Summary and discussion on degradation	14
4.2 Environmental distribution	15
4.2.1 Adsorption/desorption	15

4.2.2	Volatilisation .....	15
4.2.3	Distribution modelling .....	15
4.3	Bioaccumulation .....	15
4.3.1	Aquatic bioaccumulation .....	15
4.3.1.1	Bioaccumulation estimation .....	15
4.3.1.2	Measured bioaccumulation data .....	15
4.3.2	Terrestrial bioaccumulation .....	15
4.3.3	Summary and discussion of bioaccumulation .....	16
4.4	Secondary poisoning .....	16
5	HUMAN HEALTH HAZARD ASSESSMENT .....	16
5.1	Toxicokinetics (absorption, metabolism, distribution and elimination) .....	16
5.1.1	Non-human information .....	16
5.1.2	Human information .....	16
5.1.3	Other relevant information .....	16
5.1.4	Summary and discussion on toxicokinetics .....	17
5.2	Acute toxicity .....	17
5.2.1	Non-human information .....	17
5.2.1.1	Acute toxicity: oral .....	18
5.2.1.2	Acute toxicity: inhalation .....	18
5.2.1.3	Acute toxicity: dermal .....	18
5.2.1.4	Acute toxicity: other routes .....	18
5.2.2	Human information .....	18
5.2.3	Other relevant information .....	18
5.2.4	Summary and discussion of acute toxicity .....	19
5.3	Irritation .....	19
5.3.1	Skin .....	19
5.3.1.1	Non-human information .....	19
5.3.1.2	Human information .....	19
5.3.2	Eye .....	20
5.3.2.1	Non-human information .....	20
5.3.2.2	Human information .....	20
5.3.3	Respiratory tract .....	20
5.3.3.1	Non-human information .....	20
5.3.3.2	Human information .....	20
5.3.4	Other relevant information .....	20
5.3.5	Summary and discussion of irritation .....	20
5.4	Corrosivity .....	20
5.4.1	Non-human information .....	20
5.4.2	Human information .....	20
5.4.3	Other relevant information .....	21
5.4.4	Summary and discussion of corrosion .....	21
5.5	Sensitisation .....	21
5.5.1	Skin .....	21
5.5.1.1	Non-human information .....	21
5.5.1.2	Human information .....	21
5.5.2	Respiratory system .....	21
5.5.2.1	Non-human information .....	21
5.5.2.2	Human information .....	21
5.5.3	Other relevant information .....	21
5.5.4	Summary and discussion of sensitisation .....	22
5.5.4.1.1	Skin sensitisation .....	22
5.5.4.1.2	Respiratory sensitisation .....	22

5.5.4.1.3	Justification for classification or non classification.....	22
5.6	Repeated dose toxicity.....	22
5.6.1	Non-human information.....	22
5.6.1.1	Repeated dose toxicity: oral.....	22
5.6.1.2	Repeated dose toxicity: inhalation.....	22
5.6.1.3	Repeated dose toxicity: dermal.....	22
5.6.1.4	Repeated dose toxicity: other routes.....	22
5.6.2	Human information.....	23
5.6.3	Summary and discussion of repeated dose toxicity:.....	23
5.7	Mutagenicity.....	23
5.8	Carcinogenicity.....	23
5.9	Toxicity for reproduction.....	23
5.9.1	Effects on fertility.....	23
5.9.2	Developmental toxicity.....	24
5.10	Derivation of DNEL(s) /DMELs.....	24
5.10.1	Overview of typical dose descriptors for all endpoints.....	24
5.10.2	Correction of dose descriptors if needed (for example route-to-route extrapolation), application of assessment factors and derivation of the endpoint specific DN(M)EL.....	27
6	HUMAN HEALTH HAZARD ASSESSMENT OF PHYSICO-CHEMICAL PROPERTIES.....	28
6.1	Explosivity.....	28
6.2	Flammability.....	28
6.3	Oxidising potential.....	28
7	ENVIRONMENTAL HAZARD ASSESSMENT.....	28
7.1	Aquatic compartment (including sediment).....	28
7.1.1	Toxicity data.....	28
7.1.1.1	Fish.....	28
7.1.1.1.1	Short-term toxicity to fish.....	28
7.1.1.1.2	Long-term toxicity to fish.....	29
7.1.1.2	Aquatic invertebrates.....	29
7.1.1.2.1	Short-term toxicity to aquatic invertebrates.....	29
7.1.1.2.2	Long-term toxicity to aquatic invertebrates.....	29
7.1.1.3	Algae and aquatic plants.....	29
7.1.1.4	Sediment organisms.....	30
7.1.1.5	Other aquatic organisms.....	30
7.1.2	Calculation of Predicted No Effect Concentrations (PNEC).....	30
7.1.2.1	PNEC water (tert-butyl alcohol).....	30
7.1.2.2	PNEC sediment (tert-butyl alcohol).....	30
7.2	Terrestrial compartment.....	31
7.2.1	Calculation of Predicted No Effect Concentration (PNEC <sub>soil</sub> , tert-butyl alcohol).....	31
7.3	Atmospheric compartment.....	31
7.4	Microbiological activity in sewage treatment systems.....	32
7.4.1	Toxicity to aquatic micro-organisms (tert-butyl alcohol).....	32
7.4.2	PNEC for sewage treatment plant.....	32
7.5	Non compartment specific effects relevant for the food chain (secondary poisoning).....	33
7.5.1	Toxicity to birds.....	33

7.5.2	Toxicity to mammals.....	33
7.5.3	Calculation of PNEC <sub>oral</sub> (secondary poisoning).....	33
7.6	Conclusion on the environmental classification and labelling.....	33
8	PBT AND VPVB ASSESSMENT.....	33
8.1	Assessment of PBT/vPvB Properties – Comparison with the Criteria of Annex XIII.....	33
8.1.1	Persistence Assessment.....	33
8.1.2	Bioaccumulation Assessment.....	34
8.1.3	Toxicity Assessment.....	34
8.1.4	Summary and overall Conclusions on PBT or vPvB Properties.....	34
8.2	Emission Characterisation .....	34
9	EXPOSURE ASSESSMENT.....	35
9.1	Use 0: Production of potassium tert-butate.....	35
9.1.1	Exposure scenario.....	35
9.1.1.1	Risk management measures .....	35
9.1.1.1.1	Risk management measures related to workers.....	35
9.1.1.1.2	Risk management measures related to environment.....	36
9.1.1.1.3	Waste related measures .....	36
9.1.2	Exposure estimation .....	36
9.1.2.1	Worker exposure .....	36
9.1.2.2	Indirect exposure of humans via the environment.....	37
9.1.2.3	Environmental exposure.....	37
9.2	Use 1: Reagent in chemical synthesis.....	38
9.2.1	Exposure scenario.....	38
9.2.1.1	Risk management measures .....	39
9.2.1.1.1	Risk management measures related to workers.....	39
9.2.1.1.2	Risk management measures related to environment.....	39
9.2.1.1.3	Waste related measures .....	39
9.2.2	Exposure estimation .....	39
9.2.2.1	Worker exposure .....	39
9.2.2.2	Indirect exposure of humans via the environment.....	42
9.2.2.3	Environmental exposure.....	42
9.3	Regional and continental exposure concentrations.....	43
10	RISK CHARACTERISATION .....	43
10.1	Use 0: Production of Potassium tert-butate .....	43
10.1.1	Human health .....	43
10.1.1.1	Risk Characterisation for Workers .....	43
10.1.1.2	Indirect exposure of humans via the environment.....	44
10.1.2	Environment.....	44
10.1.2.1	Risk Characterisation (PEC/PNEC) .....	44
318	<b>Fehler! Textmarke nicht definiert.</b>	
	(DNEL <sub>long-term</sub> ) .....	45
10.2	Use 1: Reagent in chemical synthesis.....	45
10.2.1	Human health .....	45
10.2.1.1	Risk Characterisation for workers.....	45
10.2.1.2	Indirect exposure of humans via the environment.....	46
10.2.2	Environment.....	47
10.2.2.1	Risk Characterisation (PEC/PNEC) .....	47
318	47	
	(DNEL <sub>long-term</sub> ) .....	47

10.3 Overall exposure (combined for all relevant emission/release sources).....	47
10.3.1 Human health (combined for all exposure routes) .....	47
10.3.2 Environment (combined for all emission sources) .....	48
<b>REFERENCES</b> .....	49
EUROPEAN CHEMICALS AGENCY (2008) GUIDANCE DOCUMENT INFORMATION REQUIREMENTS AND CSA (R.8) .....	49



## PART A

### 1 SUMMARY OF RISK MANAGEMENT MEASURES

#### Manufacture

Use 0: Production of potassium tert-butyrate	All production processes are carried out in closed systems under inert gas atmosphere. Adequate personal protection equipment (gloves, goggles, and coverall, see SDS for details) is provided, automatic systems for sampling are used and workers are informed on potential risks.
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#### Own /Downstream use

Use 1: Reagent in chemical synthesis	All production processes are carried out in closed systems under inert gas atmosphere. Adequate personal protection equipment (gloves, goggles, and coverall, see SDS for details) is provided, automatic systems for sampling are used and workers are informed on potential risks.
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### 2 DECLARATION THAT RISK MANAGEMENT MEASURES ARE IMPLEMENTED

Risk management measures (RMM) necessary to control the risk of exposure to potassium tert-butyrate are implemented. Organisational measures are in place to ensure RMM efficiency.

### 3 DECLARATION THAT RISK MANAGEMENT MEASURES ARE COMMUNICATED

RMM are communicated via the safety data sheets (SDSs). As soon as SDSs are replaced by extended SDSs (eSDSs), RMMs will be communicated to downstream users through the eSDSs.

## PART B

### 1 IDENTITY OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Potassium tert-butyrate is a synthetic metal alcoholate with following characteristics and physical-chemical properties (see the IUCLID dataset for further details).

#### 1.1 Name and other identifiers of the substance

Table 1: Substance identity

<b>EC number:</b>	212-740-3
<b>EC name:</b>	Potassium tert-butanolate
<b>CAS number (EC inventory):</b>	865-47-4
<b>CAS number:</b>	865-47-4
<b>CAS name:</b>	Potassium tert-butanolate
<b>IUPAC name:</b>	Potassium tert-butanolate
<b>Annex I index number</b>	Not included in Annex to Directive 67/548/EEC
<b>Molecular formula:</b>	C <sub>4</sub> H <sub>9</sub> KO
<b>Molecular weight:</b>	112.2 g/mol
<b>Structural formula:</b>	(CH <sub>3</sub> ) <sub>3</sub> C-O-K

#### 1.2 Composition of the substance

Degree of purity: 100 % (for the purpose of this example, a purity of 100 % is assumed)

### 1.3 Physico-chemical properties

Table 2: Summary of physico- chemical properties

Property	Value	Remarks
Physical state at 20°C and 101.3 kPa	solid	--
Melting/freezing point	256 - 258 °C	--
Boiling point	220 °C, sublimation 270 °C, decomposition	at 1 hPa --
Relative density	not available	--
Vapour pressure	0.07 hPa	at 180 °C
Surface tension	not applicable	--
Water solubility	not applicable (decomposition)	--
Partition coefficient n-octanol/water (log value)	not applicable (decomposition)	--
Flash point	not relevant; solid	--
Flammability	highly flammable	--
Explosive properties	not explosive	--
Self-ignition temperature	360 °C	--
Oxidising properties	not oxidising	--
Granulometry	not available	--
Stability in organic solvents and identity of relevant degradation products	stable in THF, t-butanol, iso-butanol, iso-propanol	--
Dissociation constant	not available	pH of an aqueous solution of a concentration of 5 g/L is ca 13
Viscosity	not applicable, solid	--
Auto flammability	see <i>Self-ignition temperature</i> above	--
Reactivity towards container material	not available	--
Thermal stability	see <i>boiling point</i> above	--
Henry's Law constant	not relevant due to low vapour pressure	--
Stability	not stable in water or air	upon contact with water the substance decomposes spontaneously forming tert-butyl alcohol and potassium hydroxide

## 2 MANUFACTURE AND USES

### 2.1 Manufacture

Potassium tert-butyrate is manufactured adding potassium to tert-butanol. Subsequently, potassium tert-butyrate is separated and cleaned by distillation. Production takes place in closed systems under inert gas atmosphere.

A production volume of 50 tonnes / year is assumed for this CSR example.

### 2.2 Identified uses

Potassium tert-butyrate is a moderately strong base reagent that is used in many drug and chemical synthesis applications, such as alkylation, arylation, acylation, solvolysis of esters, condensation, elimination, isomerization, rearrangements, transfer hydrogenation, Wittig reactions, and redox reactions.

Use	Approximate percentage
Use 0: production	100
Use 1: reagent in chemical synthesis	100

The uses of potassium tert-butyrate in the above fields can be categorised according to VCI UEC Matrix as illustrated below, based on the following prerequisites:

- Potassium tert-butyrate is only used in industrial areas.
- Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form t-butyl alcohol and potassium hydroxide.
- Short term exposure to potassium tert-butyrate is considered relevant.
- Long term exposure to the parent compound is not considered relevant, but long term exposure to degradation products t-butyl alcohol and potassium hydroxide.
- There is no direct release to soil.

Table 3: VCI UEC Matrix for the uses of potassium tert-butyrate

Exposures	Industrial	Professional	Consumer
Human: Oral, Short-term	1	2	3
Human: Oral Long-term / Repeated	4	5	6
Human: Dermal, Short-term	7	8	9
Human: Dermal, Long-term / repeated	10	11	12
Human: Inhalation, Short-term	13	14	15
Human: Inhalation Long-term / repeated	16	17	18
Environment: Water, Single instance / Short-term	19	20	21
Environment: Water, Continuous	22	23	24
Environment: Air, Single instance / Short-term	25	26	27
Environment: Air, Continuous	28	29	30
Environment: Soil, Single instance/ Short-term	31	32	33
Environment: Soil, Continuous	34	35	36

*Use descriptions:*

### **Use 0: Production of potassium tert-butyrate**

According to the use descriptor system this use can be categorised as follows:

Sector of use:	SU3 "Industrial Manufacturing"
Product category:	Not relevant; the substance is not used in consumer products
Process categories:	PROC1 "Used in closed processes, no likelihood of exposure; industrial setting"  PROC2 "Use in closed, continuous process with occasional controlled exposure (e.g. sampling); industrial setting"
Article category:	Not relevant
Environmental release category:	Not relevant; the substance decomposes spontaneously upon contact with water or air

### **Use 1: Reagent in chemical synthesis**

According to the use descriptor system this use can be categorised as follows:

Sector of use:	SU3 "Industrial Manufacturing"
Product category:	Not relevant; the substance is not used in consumer products
Process categories:	PROC1 "Used in closed processes, no likelihood of exposure; industrial setting"  PROC2 "Use in closed, continuous process with occasional controlled exposure (e.g. sampling); industrial setting"  PROC3 "Use in closed continuous batch process (synthesis); industrial setting"  PROC4 "Use in a batch or other process (including related process stages e.g. filtration, drying) where opportunities for exposure arise (synthesis); industrial setting"
Article category:	Not relevant
Environmental release category:	Not relevant; the substance decomposes spontaneously upon contact with water or air

## **2.3 Uses advised against**

Avoid contact of potassium tert-butyrate with water or air. Potassium tert-butyrate is not to be used as such or in preparations by consumers.

**CLASSIFICATION AND LABELLING (ANNEX I OF DIRECTIVE 67/548/EEC)**

Classification and labelling of potassium tert-butyrate and its decomposition products are shown:

**3.1 Potassium tert-butyrate**

Potassium tert-butyrate is not legally classified.

**3.1.1 Self classification(s)**

Classification: F; R11 Highly flammable.  
C; R14-35 Reacts violently with water, causes severe burns  
Xn; R22 Harmful if swallowed

Labelling: F; C  
R: 11-14-22-35  
S: 8-16-26-36/37/39-43-45

Specific concentration limits

None.

**3.2 Tert-butyl alcohol**

Classification: F; R11 Highly flammable.  
Xn; R20 Harmful by inhalation

Labelling: F; Xn  
R: 11-20  
S: 9-16

Specific concentration limits

$C \geq 25 \%$  Xn, R20

**3.3 Potassium Hydroxide**

Classification: Xn; R22 Harmful if swallowed  
C; R35 Causes severe burns

Labelling: Xn; C  
R: 22-35  
S: 1/2-26-36/37/39-45

Specific concentration limits

$C \geq 25 \%$	C; R22-35
$5 \% \leq C < 25 \%$	C; R35
$2 \% \leq C < 5 \%$	C; R34
$0.5 \% \leq C < 2 \%$	Xi; R36/38

## ENVIRONMENTAL FATE PROPERTIES

### 4.1 Degradation

#### 4.1.1 Abiotic degradation

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The degradation rate in water or air is  $t_{1/2} < 120$  min.

##### 4.1.1.1 Hydrolysis

Potassium tert-butyrate: the substance hydrolyses spontaneously in contact with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The hydrolysis rate in water or air is  $t_{1/2} < 120$  min.

Tert-butyl alcohol: not applicable, the substance is readily biodegradable. Please see the IUCLID5 registration dossier for study details.

Potassium hydroxide: not applicable.

##### 4.1.1.2 Phototransformation/photolysis

General note: data on phototransformation in different media is not required by REACH.

##### 4.1.1.2.1 Phototransformation in air

Potassium tert-butyrate: not applicable.

Tert-butyl alcohol: 22 % after 15.2 hours, 50 % after 11 to 27 days (see IUCLID 5 dossier for study summary details).

Potassium hydroxide: not applicable.

##### 4.1.1.2.2 Phototransformation in water

Potassium tert-butyrate: not applicable.

Tert-butyl alcohol: 50 % after 8.8 years (see IUCLID 5 dossier for study summary details).

Potassium hydroxide: not applicable.

##### 4.1.1.2.3 Phototransformation in soil

Potassium tert-butyrate: not applicable.

Tert-butyl alcohol: no information available.

Potassium hydroxide: not applicable.

#### 4.1.2 Biodegradation

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The degradation rate in water or air is  $t_{1/2} < 120$  min.

**4.1.2.1 Biodegradation in water**

Potassium tert-butyrate: not applicable.

Tert-butyl alcohol: ready biodegradable (see IUCLID 5 dossier for study summary details).

Potassium hydroxide: not applicable.

**4.1.2.1.1 Screening tests**

The test results for tert-butyl alcohol are summarised below:

Table 4: Screening tests for biodegradation in water

Method	Degradation rate	Remarks	Reference
92/69/EC C.4	> 60 % after 10 d 99 % after 28 d	GLP	Huels Report, 2004

**4.1.2.2 Biodegradation in sediments**

Potassium tert-butyrate: not applicable.

Tert-butyl alcohol: ready biodegradable.

Potassium hydroxide: not applicable.

**4.1.2.3 Biodegradation in soil**

Potassium tert-butyrate: not applicable.

Tert-butyl alcohol: ready biodegradable.

Potassium hydroxide: not applicable.

**4.1.2.4 Summary and discussion on biodegradation**

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide.

**4.1.3 Summary and discussion on degradation**

Table 5: Biodegradation test summary

Degradation rate in water	Potassium tert-butyrate: Tert-butyl alcohol: Potassium hydroxide:	$t_{1/2} < 120$ min. ready biodegradable not applicable.
Degradation rate in sediment	Potassium tert-butyrate: Tert-butyl alcohol: Potassium hydroxide:	$t_{1/2} < 120$ min. ready biodegradable not applicable.
Degradation rate in soil	Potassium tert-butyrate: Tert-butyl alcohol: Potassium hydroxide:	$t_{1/2} < 120$ min. ready biodegradable not applicable.
Degradation rate in air	Potassium tert-butyrate: Tert-butyl alcohol: Potassium hydroxide:	$t_{1/2} < 120$ min. ready biodegradable not applicable.



## 4.2 Environmental distribution

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The degradation rate in water or air is  $t_{1/2} < 120$  min. See IUCLID 5 registration dossier for degradation product study summaries.

### 4.2.1 Adsorption/desorption

Potassium tert-butyrate: not applicable.

Tert-butyl alcohol:  $K_{oc} = 0.37$ . Please see the IUCLID5 registration dossier for study details.

Potassium hydroxide: not applicable.

### 4.2.2 Volatilisation

Potassium tert-butyrate: not applicable.

Tert-butyl alcohol: Henry's Law Constant =  $1.44 \cdot 10^{-5}$  atm m<sup>3</sup>/mol; please see the IUCLID5 registration dossier for study details.

Potassium hydroxide: not applicable.

### 4.2.3 Distribution modelling

Potassium tert-butyrate: not applicable.

Tert-butyl alcohol:	Air:	9.588 %
	Soil:	0.016 %
	Water:	90.382 %
	Sediment:	0.015 %
	Biota:	0.000 %

Please see the IUCLID5 registration dossier for study details.

Potassium hydroxide: not applicable.

## 4.3 Bioaccumulation

### 4.3.1 Aquatic bioaccumulation

#### 4.3.1.1 Bioaccumulation estimation

Potassium tert-butyrate: not applicable.

Tert-butyl alcohol: Estimated log BCF = 0.500 (BCF = 3.162) (EpiWin v3.12; Appendix I).

Potassium hydroxide: not applicable.

#### 4.3.1.2 Measured bioaccumulation data

Potassium tert-butyrate: not applicable.

Tert-butyl alcohol: log BCF = 0.036 (BCF = 1.09). Please see the IUCLID5 registration dossier for study details.

Potassium hydroxide: not applicable.

### 4.3.2 Terrestrial bioaccumulation

No data available.

#### 4.3.3 Summary and discussion of bioaccumulation

Bioaccumulation is of no concern for the parent substance and degradation products.

#### 4.4 Secondary poisoning

Secondary poisoning due to bioaccumulation in organisms is of no concern for the parent substance or its degradation products.

### 5 HUMAN HEALTH HAZARD ASSESSMENT

#### 5.1 Toxicokinetics (absorption, metabolism, distribution and elimination)

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The degradation rate in water or air is  $t_{1/2} < 120$  min. The degradation reactions may be violent (therefore labelling with R14; reacts violently with water). Due to the reactive nature of the substance, potassium tert-butyrate may potentially cause significantly adverse local effects (R35; causes severe burns). However, even though potassium tert-butyrate may potentially cause adverse local effects, there is practically no systemic toxicity. Potassium tert-butyrate does not become bioavailable, as the substance decomposes before absorption can occur.

Instead, the systemic toxicological profile of potassium tert-butyrate is determined by its degradation products. Potentially significant toxicological effects are caused by tert-butyl alcohol. The second degradation product, potassium hydroxide, can cause significant local effects (corrosive, R35; causes severe burns), but contributes only little to the systemic toxicological profile, as the substance is of reactive nature (very strong base) and the potassium ion is an essential mineral micronutrient in human nutrition. The 2004 guidelines of the US National Institute of Medicine specify a recommended dietary allowance (RDA) of 4,700.00 mg of potassium (National Academy of Sciences, 2002).

Several toxicokinetic studies using different species on tert-butyl alcohol are included in the IUCLID5 registration dossier. A summary of the toxicokinetic profile of tert-butyl alcohol is provided in section 5.1.4.

##### 5.1.1 Non-human information

Potassium tert-butyrate: not applicable.

Tert-butyl alcohol: please refer to study summaries in the IUCLID 5 registration dossier.

Potassium hydroxide: not applicable.

##### 5.1.2 Human information

Potassium tert-butyrate: not applicable.

Tert-butyl alcohol: please refer to study summaries in the IUCLID 5 registration dossier.

Potassium hydroxide: not applicable.

##### 5.1.3 Other relevant information

Potassium tert-butyrate: not applicable.

Tert-butyl alcohol: please refer to study summaries in the IUCLID 5 registration dossier.  
Potassium hydroxide: not applicable.

#### 5.1.4 Summary and discussion on toxicokinetics

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The degradation rate in water or air is  $t_{1/2} < 120$  min. The degradation reactions may be violent (therefore labelling with R14; reacts violently with water) and due to the reactive nature of the substance, potassium tert-butyrate may potentially cause significantly adverse local effects (R35; causes severe burns).

However, even though potassium tert-butyrate may potentially cause adverse local effects, there is practically no systemic toxicity. Potassium tert-butyrate does not become bioavailable, as decomposition occurs before the substance is absorbed. Instead, the systemic toxicological profile of potassium tert-butyrate is determined by its degradation products, with potentially significant toxicological effects caused by tert-butyl alcohol. The degradation product potassium hydroxide does not contribute to the systemic toxicological profile of potassium tert-butyrate. However, as the substance is reactive in nature (corrosive, R35; causes severe burns), additional local effects can be expected.

Following exposure potassium tert-butyrate decomposes upon contact with animal or human tissue, producing potassium hydroxide and tert-butyl alcohol. Potassium hydroxide further reacts with tissues to form potassium ions ( $K^+$ ) and water. Potassium is an essential mineral micronutrient in human nutrition. The 2004 guidelines of the US National Institute of Medicine specify a recommended dietary allowance (RDA) of 4,700.00 mg of potassium (National Academy of Sciences, 2002).

The second decomposition product, tert-butyl alcohol, is rapidly absorbed following oral or inhalation exposure. Absorption following dermal exposure is negligible, due to the compounds physical-chemical properties. After absorption, tert-butyl alcohol is likely to be metabolised and the substance and its metabolites are distributed throughout body fluids and organs. The substance is not likely to bioconcentrate, based on the measured and estimated BCFs of 1.09 and 3.16, respectively.

Several phase I metabolic reactions, catalysed by cytochrome P-450-dependent monooxygenase enzymes may occur. Parent compound and metabolites formed in phase I metabolic reactions may be rendered more polar by phase II metabolism. Finally, remaining amounts of the parent compound and formed metabolites are expected to be excreted in urine or bile and faeces. The half-life of tert-butyl alcohol in blood at several dose levels is ca. 9 to 13 hours.

Pharmacokinetics of tert-butyl alcohol were shown to be indifferent to the route of uptake.

#### 5.2 Acute toxicity

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The degradation rate in water or air is  $t_{1/2} < 120$  min. Thus, whilst local effects may occur due to the parent compound and the degradation product potassium hydroxide, systemic toxicity is mainly attributed to the degradation product tert-butyl alcohol.

##### 5.2.1 Non-human information

Please refer to the IUCLID 5 registration dossier for study summaries.

**5.2.1.1 Acute toxicity: oral**

Potassium tert-butyrate: LD<sub>50</sub> (rat): 690 mg/kg bw. See the IUCLID5 registration dossier for study summary details.

→ R22, harmful if swallowed.

Tert-butyl alcohol: LD<sub>50</sub> (rat): 2733 - 3046 mg/kg bw. See the IUCLID5 registration dossier for study summary details.

Potassium hydroxide: LD<sub>50</sub> (rat): 27 - 1890 mg/kg bw. See the IUCLID5 registration dossier for study summary details.

→ R22, harmful if swallowed.

**5.2.1.2 Acute toxicity: inhalation**

Potassium tert-butyrate: no data are available; due to the substance's high reactivity severe local effects are expected.

Tert-butyl alcohol: LD<sub>50</sub> (rat): > 10,000 ppm/4 h (> 30,316 mg/m<sup>3</sup>/4 h). See the IUCLID5 registration dossier for study summary details.

Potassium hydroxide: due to the substance's high reactivity severe local effects are expected.

**5.2.1.3 Acute toxicity: dermal**

Potassium tert-butyrate: due to the substance's high reactivity no systemic, but severe local effects are expected.

Tert-butyl alcohol: LD<sub>50</sub> (rat): > 2000 mg/kg bw. See the IUCLID5 registration dossier for study summary details.

Potassium hydroxide: due to the substance's high reactivity no systemic, but severe local effects are expected.

**5.2.1.4 Acute toxicity: other routes**

No data available.

**5.2.2 Human information**

Potassium tert-butyrate: no information available.

Tert-butyl alcohol: Classification as harmful by inhalation based on human data. See the IUCLID5 registration dossier for study summary details.

→ R20, harmful by inhalation.

Potassium hydroxide: no information available.

**5.2.3 Other relevant information**

None.

### 5.2.4 Summary and discussion of acute toxicity

Table 6: Acute dose toxicity test summary

Endpoint	Quantitative dose descriptor		Associated relevant effect	Remarks on study
	Local effects	Systemic effects		
Acute toxicity Oral	Potassium tert-butyrate may cause local effects, due to its high reactivity	Potassium tert-butyrate: LD <sub>50</sub> (rat): 690 mg/kg bw → R22; Harmful if swallowed Tert-butyl alcohol: LD <sub>50</sub> (rat): 2733 - 3046 mg/kg bw. Potassium hydroxide: LD <sub>50</sub> (rat): 27 - 1890 mg/kg bw	Mortality	Several studies in mammals, with and without information on GLP
Acute toxicity Inhalation	Potassium tert-butyrate may cause local effects, due to its high reactivity	Potassium tert-butyrate: -- Tert-butyl alcohol: LD <sub>50</sub> (rat): > 10,000 ppm/4 h (> 30,316 mg/m <sup>3</sup> /4 h) Potassium hydroxide: --	Mortality	-- GLP study --
Acute toxicity Dermal	Potassium tert-butyrate may cause local effects, due to its high reactivity	Potassium tert-butyrate: -- Tert-butyl alcohol: LD <sub>50</sub> (rat): > 2000 mg/kg bw Potassium hydroxide: --	Mortality	-- GLP study --

The LD<sub>50</sub> of potassium tert-butyrate is 690 mg/kg bw requiring classification as R22, harmful if swallowed. No data on acute inhalation and dermal toxicity are available for potassium tert-butyrate. However, based on the reactivity of potassium tert-butyrate severe local findings are expected. With the exception of the acute oral toxicity values for potassium hydroxide, resulting in classification as R22, harmful if swallowed, all other acute toxicity LD<sub>50</sub>-values for degradation products exceed limit concentrations. Classification of tert-butyl alcohol as R20, harmful by inhalation, is based on human data.

## 5.3 Irritation

Please refer to the IUCLID 5 registration dossier for study summaries.

### 5.3.1 Skin

#### 5.3.1.1 Non-human information

Potassium tert-butyrate: in a study on rabbits (OECD 404) potassium tert-butyrate caused severe burns.

→ Corrosive, R35; causes severe burns.

Tert-butyl alcohol: not irritating.

Potassium hydroxide: caused severe burns.

→ Corrosive, R35; causes severe burns.

#### 5.3.1.2 Human information

No data available.

**5.3.2 Eye****5.3.2.1 Non-human information**

No data available; based on the reactivity of potassium tert-butyrate and the degradation product potassium hydroxide with water or air, severe local findings are expected.

**5.3.2.2 Human information**

No data available.

**5.3.3 Respiratory tract****5.3.3.1 Non-human information**

No data available; based on the reactivity of potassium tert-butyrate and the degradation product potassium hydroxide with water or air no systemic, but severe local findings are expected.

**5.3.3.2 Human information**

No data available; based on the reactivity of potassium tert-butyrate and the degradation product potassium hydroxide with water or air no systemic, but severe local findings are expected.

**5.3.4 Other relevant information**

No data available.

**5.3.5 Summary and discussion of irritation**

A skin irritation test (OECD 404) showed that Potassium tert-butyrate caused severe skin burns. In addition the degradation product potassium hydroxide also caused severe burns when applied to the skin.

→ Corrosive, R35; causes severe burns.

**5.4 Corrosivity**

A skin irritation test (OECD 404) showed that Potassium tert-butyrate caused severe skin burns. In addition the degradation product potassium hydroxide also caused severe burns when applied to the skin.

→ Corrosive, R35; causes severe burns.

**5.4.1 Non-human information**

See statement under section 5.4.

**5.4.2 Human information**

See statement under section 5.4.

**5.4.3 Other relevant information**

None.

**5.4.4 Summary and discussion of corrosion**

See statement under section 5.4.

**5.5 Sensitisation**

Please refer to the IUCLID 5 registration dossier for study summaries.

**5.5.1 Skin****5.5.1.1 Non-human information**

Potassium tert-butyrate: no data available, skin sensitisation is not expected (corrosive, R35; causes severe burns).

Tert-butyl alcohol: Study on guinea pigs (OECD 406, GPMT): not sensitising. Please refer to the IUCLID 5 registration dossier for study summaries.

Potassium hydroxide: no data available, skin sensitisation is not expected (R35; causes severe burns).

**5.5.1.2 Human information**

No data available. Based on the reactivity of potassium tert-butyrate with water and the results of the skin irritation tests severe local findings are expected. Skin sensitisation is not expected.

**5.5.2 Respiratory system**

No data available. Based on the reactivity of potassium tert-butyrate with water and the results of the skin irritation tests severe local findings are expected. Respiratory tract sensitisation is not expected.

**5.5.2.1 Non-human information**

See statement under section 5.5.2.

**5.5.2.2 Human information**

See statement under section 5.5.2.

**5.5.3 Other relevant information**

No data available.

## 5.5.4 Summary and discussion of sensitisation

### 5.5.4.1.1 Skin sensitisation

No sensitisation expected based on the corrosive properties of potassium tert-butyrate and its degradation product potassium hydroxide. Tert-butyl alcohol was shown to be non-sensitising.

### 5.5.4.1.2 Respiratory sensitisation

No sensitisation expected based on the corrosive properties of potassium tert-butyrate and its degradation product potassium hydroxide. Tert-butyl alcohol was shown to be no skin sensitizer. Therefore, it is expected that tert-butyl alcohol does not elicit respiratory sensitisation.

### 5.5.4.1.3 Justification for classification or non classification

Not classified.

## 5.6 Repeated dose toxicity

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The degradation rate in water or air is  $t_{1/2} < 120$  min. Thus, toxicity is mainly attributed to degradation products.

### 5.6.1 Non-human information

#### 5.6.1.1 Repeated dose toxicity: oral

Potassium tert-butyrate: no information available.

Tert-butyl alcohol: several sub-chronic (90-day) and chronic repeated oral toxicity studies are available. The observations in chronic studies support the findings in subchronic studies. See the IUCLID 5 registration dossier for study summaries.

Potassium hydroxide: no information available.

#### 5.6.1.2 Repeated dose toxicity: inhalation

Potassium tert-butyrate: no information available.

Tert-butyl alcohol: several repeated sub-chronic (90-day) inhalation toxicity studies are available. See the IUCLID 5 registration dossier for study summaries.

Potassium hydroxide: no information available.

#### 5.6.1.3 Repeated dose toxicity: dermal

No information available.

#### 5.6.1.4 Repeated dose toxicity: other routes

No information available.



### 5.6.2 Human information

No information available.

### 5.6.3 Summary and discussion of repeated dose toxicity:

Table 7: Repeated dose toxicity test summary

Endpoint	Quantitative dose descriptor (appropriate unit) or qualitative assessment		Associated relevant effect	Remarks on study
	Local effects	Systemic effects <sup>1</sup>		
Repeated dose toxicity Sub-chronic Oral	Due to its high reactivity local effects are expected with potassium tert-butylate	Potassium tert-butylate: -- Tert-butyl alcohol: NOAEL = 235.4 mg/kg bw/day (0.25 % in drinking water)  Potassium hydroxide: --	-- Tert-butyl alcohol: Reduced body weight gain at 0.5 %  --	Fischer 344 rats, 90 d: 0.25, 0.5, 1.0, 2.0 and 4.0 % in drinking water
Repeated dose toxicity Sub-chronic Dermal	Due to its high reactivity local effects are expected with potassium tert-butylate	Potassium tert-butylate: -- Tert-butyl alcohol: Derived from repeated oral toxicity: 235.4 mg/kg bw/day <sup>2</sup> Potassium hydroxide: --	--  -- --	Derived from repeated oral toxicity with 100% absorption assumed
Repeated dose toxicity Sub-chronic Inhalation	Due to its high reactivity local effects are expected with potassium tert-butylate	Potassium tert-butylate: -- Tert-butyl alcohol: NOAEL = 2100 ppm (6366 mg/m <sup>3</sup> )  Potassium hydroxide: --	-- Tert-butyl alcohol: No adverse findings at the highest dose  --	Fischer 344 rats, 90 d: 136, 270, 540, 1080, 2100 ppm 6 h/d 5 d/wk

<sup>1</sup>The results of the key studies are supported by findings in chronic studies

<sup>2</sup>Calculated according to Guidance Document Information Requirements and CSA (R.8), 2008

## 5.7 Mutagenicity

Potassium tert-butylate: no information available.

Tert-butyl alcohol: Negative results obtained in *in vitro* Ames tests, a mouse lymphoma assay and a sister chromatid exchange assay, see IUCLID 5 registration dossier for details. According to Annex I of EU Directive 67/548/EEC the substance is not classified as mutagenic.

Potassium hydroxide: no information available.

## 5.8 Carcinogenicity

Potassium tert-butylate: no information available.

Tert-butyl alcohol: one dermal study carried out in mice, using a 16.6 % solution in benzene and pre-treatment with 4-nitroquinoline (no standard study; initiation-promotion test), see IUCLID 5 registration dossier for details. No classification proposed.

Potassium hydroxide: no information available.

## 5.9 Toxicity for reproduction

### 5.9.1 Effects on fertility

Potassium tert-butylate: no information available.

Tert-butyl alcohol: No findings with respect to reproduction organs were observed in any of the sub-chronic studies.

Potassium hydroxide: no information available.

### **5.9.2 Developmental toxicity**

Potassium tert-butyrate: no information available.

Tert-butyl alcohol: Several studies are available. Key study: a rat inhalation study using > 99% pure substance revealed a maternal NOAEL = 2000 ppm and for the offspring a NOAEL  $\geq$  5000 ppm.

Please see the IUCLID 5 registration dossier for details. No classification is proposed.

Potassium hydroxide: no information available.

## **5.10 Derivation of DNEL(s) /DMELs**

### **5.10.1 Overview of typical dose descriptors for all endpoints**

In table 11 relevant information on potassium tert-butyrate toxicity as well as toxicity of degradation products, is summarised. Two DNELs are derived:

- DNEL<sub>acute</sub>
- DNEL<sub>long-term</sub>

Table 8: Available dose-descriptor(s) per endpoint for potassium tert-butyrate as a result of its hazard assessment.

Endpoint		Quantitative dose descriptor (appropriate unit) or qualitative assessment		Associated relevant effect	Remarks on study
		Local	Systemic		
Acute toxicity	oral	Potassium tert-butyrate and potassium hydroxide may cause local effects, due to their reactivity	Potassium tert-butyrate: LD <sub>50</sub> (rat): 690 mg/kg bw → R22; Harmful if swallowed Tert-butyl alcohol: LD <sub>50</sub> (rat): 2733 - 3046 mg/kg bw Potassium hydroxide: LD <sub>50</sub> (rat): 27 - 1890 mg/kg bw	Mortality  Mortality  Mortality	Several studies in mammals, with and without information on GLP status
	dermal	Potassium tert-butyrate and potassium hydroxide may cause local effects, due to their reactivity	Potassium tert-butyrate: -- Tert-butyl alcohol: LD <sub>50</sub> (rat): > 2000 mg/kg bw Potassium hydroxide: --	--  Mortality  --	--  GLP study  --
	inhalation	Potassium tert-butyrate and potassium hydroxide may cause local effects, due to their reactivity	Potassium tert-butyrate: -- Tert-butyl alcohol: LD <sub>50</sub> (rat): > 10,000 ppm/4 h (> 30,316 mg/m <sup>3</sup> /4 h) Potassium hydroxide: --	--  Mortality  --	--  GLP study  --
Irritation/Corrosivity	skin	Potassium tert-butyrate: Causes severe burns → Corrosive, R 35 causes severe burns Tert-butyl alcohol: not irritating Potassium hydroxide: Causes severe burns → Corrosive, R 35 causes severe burns		Irritation/Corrosion	→ Corrosive, R 35 causes severe burns  --  → Corrosive, R 35 causes severe burns
	eye	Potassium tert-butyrate: Severe eye damage expected Tert-butyl alcohol: not irritating Potassium hydroxide: Severe eye damage expected		--	
	Respiratory tract	Potassium tert-butyrate and potassium hydroxide may cause local effects, due their reactivity		--	
Sensitisation	skin	--  --	Potassium tert-butyrate: skin sensitisation not expected. Tert-butyl alcohol: not sensitising. Potassium hydroxide: skin sensitisation not expected.	--  --	--  Tert-butyl alcohol: GPMT (OECD 406)
	Respiratory tract	--	Potassium tert-butyrate: respiratory sensitisation not expected. Tert-butyl alcohol: respiratory sensitisation not expected. Potassium hydroxide: respiratory sensitisation not expected.	--  --	--  --
		--	--	--	--

Endpoint		Quantitative dose descriptor (appropriate unit) or qualitative assessment		Associated relevant effect	Remarks on study
		Local	Systemic		
Repeated dose toxicity (Sub)-Chronic (derived on the basis of a sub-chronic mice and a chronic rat study)	oral	Potassium tert-butyrate and potassium hydroxide may cause local effects	Potassium tert-butyrate: -- Tert-butyl alcohol: NOAEL = 235.4 mg/kg bw/day (0.25 % in drinking water)  Potassium hydroxide: --	-- Reduced body weight gain at 0.5 %  --	-- Tert-butyl alcohol: Fischer 344 rats, 90 d: 0.25, 0.5, 1.0, 2.0 and 4.0 % in drinking water  --
	dermal	Potassium tert-butyrate and potassium hydroxide may cause local effects		--	
	inhalation	Potassium tert-butyrate and potassium hydroxide may cause local effects	Potassium tert-butyrate: -- Tert-butyl alcohol: NOAEL = 2,100 ppm (6,366 mg/m <sup>3</sup> )  Potassium hydroxide: --	-- No adverse findings observed at the highest dose (2,100 ppm)  --	-- Tert-butyl alcohol: Fischer 344 rats, 90 d: 136, 270, 540, 1080, 2100 ppm 6 h/d 5 d/wk → R20, Harmful by inhalation (local effects)  --
	in vivo	--	--	--	--
Mutagenicity	in vitro	--  --	Potassium tert-butyrate: -- Tert-butyl alcohol: Not mutagenic  Potassium hydroxide: --	--  --	-- Tert-butyl alcohol: Negative results obtained in <i>in vitro</i> Ames tests, a mouse lymphoma assay and a sister chromatid exchange assay  --
		--	--	--	--
Carcinogenicity	oral	--	--	--	--
	dermal	--  --	Potassium tert-butyrate: -- Tert-butyl alcohol: 16.6 % in benzene; dermal study in mice Potassium hydroxide: --	--  --	-- Tert-butyl alcohol: no standard study (initiation-promotion test); not carcinogenic  --
	inhalation	--	--	--	--
Reproductive toxicity fertility impairment	oral			--	--
	dermal			--	--
	inhalation			--	-- Tert-butyl alcohol: No relevant effects observed in any of the subchronic studies --
Reproductive toxicity developmental toxicity	oral	--	--	--	--
	dermal	--	--	--	--
	inhalation	--  --	Potassium tert-butyrate: -- Tert-butyl alcohol: Maternal NOAEL = 2000 ppm Offspring NOAEL ≥ 5000 ppm Potassium hydroxide: --	--  --	-- Tert-butyl alcohol: > 99% pure substance  --

### 5.10.2 Correction of dose descriptors if needed (for example route-to-route extrapolation), application of assessment factors and derivation of the endpoint specific DN(M)EL

For simplification, table 8 was adapted. Only systemic effects were considered as, besides the corrosive effects, no other relevant local effects occurred in studies compiled. Exposure to potassium tert-butyrate does not lead to bioavailability of the compound as such. Instead, following exposure potassium tert-butyrate decomposes upon contact with animal or human tissue, producing potassium hydroxide and tert-butyl alcohol. Potassium hydroxide further reacts to form potassium ions ( $K^+$ ) and water. Therefore, the parent compound and the decomposition product potassium hydroxide are of minor toxicological importance with respect to systemic/long-term toxicity. The systemic toxicity profile of potassium tert-butyrate is determined by tert-butyl alcohol. The dose descriptors of the decomposition product tert-butyl alcohol are used for those endpoints, for which no data on the parent compound are available. No DNELs were derived for mutagenicity, carcinogenicity, reprotoxicity, developmental toxic as potassium tert-butyrate or its decomposition products were not mutagenic, carcinogenic, reprotoxic or developmental toxic. Hence, table 9 shows acute and long-term DNELs as related to systemic toxicity. DNELs were adjusted for allometric scaling from rats to humans, respiratory volume at light activity and intraspecies differences (workers).

Table 9: Corrected dose descriptor(s) per endpoint and endpoint-specific worst case DNEL(s)/DMEL(s) appropriate for all exposure patterns

Endpoint		Most relevant quantitative dose descriptor (appropriate unit)	Overall AF applied	Endpoint-specific DNEL/DMEL (appropriate unit)
Acute toxicity	oral	Potassium tert-butyrate: LD <sub>50</sub> (rat): 690 mg/kg bw	Allometric scaling: 4 Intraspecies (worker): 5 Total: 20	DNEL <sub>acute, oral</sub> = 34.5 mg/kg bw
	dermal	Tert-butyl alcohol determines dermal toxicity: LD <sub>50</sub> (rat): > 2000 mg/kg bw	Allometric scaling: 4 Intraspecies (worker): 5 Total: 20	DNEL <sub>acute, dermal</sub> = 34.5 mg/kg bw
	inhalation (4 hour)	Tert-butyl alcohol determines inhalation toxicity: LD <sub>50</sub> (rat): > 10,000 ppm/4 h (> 30,316 mg/m <sup>3</sup> /4 h)	Adjusted for light activity: 1.5 Intraspecies (worker): 5 Total: 7.5	DNEL <sub>acute, inhal</sub> = 1,333 ppm (4042 mg/m <sup>3</sup> )
Repeated dose toxicity (subchronic findings are supported by chronic studies, thus no assessment factor for duration needs to be applied)	oral	Tert-butyl alcohol determines oral toxicity: NOAEL = 235.4 mg/kg bw/day	Allometric scaling: 4 Intraspecies (worker): 5 Total: 20	DNEL <sub>long-term, oral</sub> = 11.72 mg/kg bw/day
	dermal	Based on the sub-chronic oral toxicity of potassium tert-butyrate: NOAEL = 235.4 mg/kg bw/day	Allometric scaling: 4 Intraspecies (worker): 5 Total: 20	DNEL <sub>long-term, dermal</sub> = 11.72 mg/kg bw/day
	inhalation	Tert-butyl alcohol determines inhalation toxicity: NOAEL = 2100 ppm (6366 mg/m <sup>3</sup> )	Adjusted for light activity: 1.5 Intraspecies (worker): 5 Total: 7.5	DNEL <sub>long-term, inhal</sub> = 280 ppm (849 mg/m <sup>3</sup> )

## **6 HUMAN HEALTH HAZARD ASSESSMENT OF PHYSICO-CHEMICAL PROPERTIES**

### **6.1 Explosivity**

Potassium tert-butyrate is not explosive.

### **6.2 Flammability**

Potassium tert-butyrate is highly flammable.

→ R11, highly flammable.

### **6.3 Oxidising potential**

Potassium tert-butyrate is not oxidising.

## **7 ENVIRONMENTAL HAZARD ASSESSMENT**

### **7.1 Aquatic compartment (including sediment)**

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The degradation rate in water or air is  $t_{1/2} < 120$  min. The reaction with water is violent (R14; reacts violently with water). Therefore, there is practically no exposure of potassium tert-butyrate to the aquatic environment. Thus, potassium tert-butyrate cannot have any significant toxicological effect on the aquatic environment. Instead the decomposition products potassium hydroxide and tert-butyl alcohol need to be considered.

The hydrolysis product potassium hydroxide further reacts with water/(organic) acids to produce potassium ions and water. Potassium is the seventh most abundant element, present as various compounds, making up about 1.5 % of the weight of the Earth's crust (Winter, 2008). Therefore, potassium hydroxide is not considered relevant for this assessment.

The environmental effects profile of potassium tert-butyrate is not determined by the substance itself. Instead, effects are determined by the decomposition product tert-butyl alcohol. In the following sections, aquatic toxicity data for tert-butyl alcohol is shown.

#### **7.1.1 Toxicity data**

##### **7.1.1.1 Fish**

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. Toxicity to fish may be potentially caused by tert-butyl alcohol.

##### **7.1.1.1.1 Short-term toxicity to fish**

Tert-butyl alcohol results are summarised in table 10. Study summaries are included in the IUCLID 5 registration dossier.

Table 10: Summary of tert-butyl alcohol short-term effects on fish

Species	Results	Remarks	Reference
Brachydanio rerio	NOEC $\geq$ 856 mg/L	92/69/EEC C.1, GLP	Huels Report, 1994

**7.1.1.1.2** Long-term toxicity to fish

No data on the long-term toxicity to fish available.

**7.1.1.2 Aquatic invertebrates**

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. Toxicity to invertebrates may be potentially caused by tert-butyl alcohol.

**7.1.1.2.1** Short-term toxicity to aquatic invertebrates

Tert-butyl alcohol results are summarised in table 11. Study summaries are included in the IUCLID 5 registration dossier.

Table 11: Summary of tert-butyl alcohol short-term effects on invertebrates

Species	Results	Remarks	Reference
Daphnia magna	NOEC = 180 mg/L EC50(48 h) = 933 mg/L	92/69/EEC C.2, GLP	Huels Report, 1994

**7.1.1.2.2** Long-term toxicity to aquatic invertebrates

No data on the long-term toxicity to aquatic invertebrates available.

**7.1.1.3 Algae and aquatic plants**

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. Toxicity to invertebrates may be potentially caused by tert-butyl alcohol.

Tert-butyl alcohol results are summarised in table 12. Study summaries are included in the IUCLID 5 registration dossier.

Table 12: Summary of tert-butyl alcohol effects on algae and aquatic plants

Species	Results	Remarks	Reference
<i>Scenedesmus subspicatus</i>	NOEC > 1000 mg/L (biomass); EC 50 > 1000 mg/L (growth rate)	92/69/EEC C.2, GLP	Huels Report, 1994

#### 7.1.1.4 Sediment organisms

No data available. The PNEC for sediment is derived via the equilibrium partitioning method based on the  $PNEC_{\text{aquatic}}$ .

#### 7.1.1.5 Other aquatic organisms

### 7.1.2 Calculation of Predicted No Effect Concentrations (PNEC)

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The degradation rate in water or air is  $t_{1/2} < 120$  min. The reaction with water is violent (R14; reacts violently with water). Therefore, there is practically no exposure of potassium tert-butyrate to the aquatic environment. Thus, potassium tert-butyrate cannot have any significant toxicological effect on the aquatic environment. Instead the decomposition products potassium hydroxide and tert-butyl alcohol need to be considered.

The hydrolysis product potassium hydroxide further reacts with water/(organic) acids to produce potassium ions and water. Potassium is the seventh most abundant element, present as various compounds, making up about 1.5% of the weight of the Earth's crust (Winter, 2008). Therefore, potassium hydroxide is not considered relevant for this assessment.

The environmental effects profile of potassium tert-butyrate is not determined by the substance itself. Instead, effects are determined by the decomposition product tert-butyl alcohol. Therefore PNEC-values are calculated for tert-butyl alcohol.

#### 7.1.2.1 PNEC water (tert-butyl alcohol)

The lowest effect concentrations were observed for aquatic invertebrates (*Daphnia magna*), with a 48 hour  $EC_{50}$ (48 h) of 933 mg/L. The TGD (2003) suggest applying an assessment factor of 100 to the lowest end of the acute toxicity range (933 mg/l), taking into account the ready biodegradability of the substance. This results in a PNEC for aquatic organisms of 9.3 mg/l.

$$PNEC_{\text{aquatic organisms}} = \text{lowest end acute toxicity range}/100 = 9.3 \text{ mg/l}$$

The data set only includes freshwater species. Therefore, in absence of data on saltwater species, the above PNEC is used for both, freshwater and marine environments.

#### 7.1.2.2 PNEC sediment (tert-butyl alcohol)

An estimation of the PNEC sediment can be performed according to the equilibrium partitioning method according to the following equation:

$$PNEC_{\text{sediment}} = (K_{\text{susp-water}} / RHO_{\text{susp}}) * PNEC_{\text{water}} * 1000$$

$$\text{According to EUSES: } K_{\text{susp-water}} = 1.27 \text{ m}^3/\text{m}^3$$

$$\text{According to the "R16" Guidance document equation R16-13: } RHO_{\text{susp}} = 1150 \text{ kg/m}^3$$

$$\rightarrow PNEC_{\text{sediment}} = (1.27 / 1150) * PNEC_{\text{water}} * 1000 = 10.3 \text{ mg/kg}$$

This estimation indicates that there is no concern for the sediment, when compared to the aquatic compartment, as PNEC-values are higher. Therefore, no further testing of the toxicity of potassium tert-butyrate to sediment organisms is required.



## 7.2 Terrestrial compartment

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The degradation rate in water or air is  $t_{1/2} < 120$  min. The reaction with water is violent (R14; reacts violently with water). Therefore, there is practically no exposure of potassium tert-butyrate to the environment. Thus, potassium tert-butyrate cannot have any significant toxicological effect on the terrestrial compartment. Instead the decomposition products potassium hydroxide and tert-butyl alcohol need to be considered.

The hydrolysis product potassium hydroxide further reacts with water/(organic) acids to produce potassium ions and water. Potassium is the seventh most abundant element, present as various compounds, making up about 1.5% of the weight of the Earth's crust (Winter, 2008). Therefore, potassium hydroxide is not considered relevant for this assessment.

The environmental effects profile of potassium tert-butyrate is not determined by the substance itself. Instead, effects are determined by the decomposition product tert-butyl alcohol. Therefore PNEC-values are calculated for tert-butyl alcohol.

As tert-butyl alcohol is readily biodegradable, effects on soil organisms are not considered. Due to the low tendency to adsorb to solid matter and the resulting low tendency to adsorb to sewage sludge, which might be deposited onto soil, the indirect exposure of soil to tert-butyl alcohol via sewage sludge is also of no concern.

### 7.2.1 Calculation of Predicted No Effect Concentration (PNEC<sub>soil</sub>, tert-butyl alcohol)

The PNEC<sub>soil</sub> can be estimated via the equilibrium partitioning method:

$$\text{PNEC}_{\text{soil}} = (K_{\text{soil-water}} / \text{RHO}_{\text{soil}}) * \text{PNEC}_{\text{water}} * 1000$$

$$\text{According to EUSES: } K_{\text{soil-water}} = 0.3 \text{ m}^3 / \text{m}^3$$

$$\text{According to the "R16" Guidance document equation R16-23: } \text{RHO}_{\text{soil}} = 1700 \text{ kg/m}^3$$

$$\rightarrow \text{PNEC}_{\text{soil}} = (0.3 / 1700) * \text{PNEC}_{\text{water}} * 1000 = 16.4 \text{ mg/kg}$$

This estimation indicates that there is no concern for the soil compartment, when compared to the aquatic compartment and that therefore no further testing of the toxicity of tert-butyl alcohol to soil organisms is necessary.

## 7.3 Atmospheric compartment

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The degradation rate in water or air is  $t_{1/2} < 120$  min. The reaction with water is violent (R14; reacts violently with water). Therefore, there is practically no exposure of potassium tert-butyrate to the environment. Thus, potassium tert-butyrate cannot have any significant toxicological effect on the atmospheric compartment. Instead the decomposition products potassium hydroxide and tert-butyl alcohol need to be considered.

The hydrolysis product potassium hydroxide further reacts with water/(organic) acids to produce potassium ions and water. Potassium is the seventh most abundant element, present as various compounds, making up about 1.5% of the weight of the Earth's crust (Winter, 2008). Therefore, potassium hydroxide is not considered relevant for this assessment.

The environmental effects profile of potassium tert-butyrate is not determined by the substance itself. Instead, effects are determined by the decomposition product tert-butyl alcohol. Therefore PNEC-values are calculated for tert-butyl alcohol.

For tert-butyl alcohol the highest  $PEC_{air}$ -value, as calculated in EUSES, is  $2.45 \cdot 10^{-6} \text{ mg/m}^3$  which is ca. 8 orders of magnitudes below the tert-butyl alcohol long term inhalative DNEL of  $343 \text{ mg/m}^3$  (see Appendix II). This comparison indicates that exposure of atmospheric biota to tert-butyl alcohol via the atmosphere is of no concern.

Further, there is no structural alert in the chemical structure of tert-butyl alcohol to expect effects on global warming, ozone depletion in the stratosphere, ozone formation in the troposphere or acidification.

#### 7.4 Microbiological activity in sewage treatment systems

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The degradation rate in water or air is  $t_{1/2} < 120 \text{ min}$ . The reaction with water is violent (R14; reacts violently with water). Therefore, there is practically no exposure of potassium tert-butyrate to the environment. Thus, potassium tert-butyrate cannot have any significant toxicological effect on the atmospheric compartment. Instead the decomposition products potassium hydroxide and tert-butyl alcohol need to be considered.

The hydrolysis product potassium hydroxide further reacts with water/(organic) acids to produce potassium ions and water. Potassium is the seventh most abundant element, present as various compounds, making up about 1.5% of the weight of the Earth's crust (Winter, 2008). Therefore, potassium hydroxide is not considered relevant for this assessment.

The environmental effects profile of potassium tert-butyrate is not determined by the substance itself. Instead, effects are determined by the decomposition product tert-butyl alcohol. Therefore PNEC-values are calculated for tert-butyl alcohol.

##### 7.4.1 Toxicity to aquatic micro-organisms (tert-butyl alcohol)

Results for tert-butyl alcohol are summarised in table 13. Study summaries are included in the IUCLID 5 registration dossier.

Table 13: Summary of effects on micro-organisms

Species	Results	Remarks	Reference
<i>Pseudomonas putida</i>	EC10 = 6,900 mg/L EC50 > 10,000 mg/L	17 hour exposure period	Huels Report, 1994

Guidance Document Information Requirements and CSA (2008) suggests the application of the factor 10 to the  $EC_{50}$  and one to the NOEC, if the test was performed with nitrifying bacteria. This is the case for *Pseudomonas* species. For e.g. respiration inhibition or similar endpoints, an assessment factor of 100 would have to be used. Therefore,

$$PNEC_{\text{microorganisms}} = 1,000 \text{ mg/l}$$

##### 7.4.2 PNEC for sewage treatment plant

The  $PNEC_{STP}$  is derived on the basis of the  $PNEC_{\text{microorganisms}}$  (see section 7.4.1):

$$PNEC_{STP} = 1,000 \text{ mg/l}$$

### 7.5 Non compartment specific effects relevant for the food chain (secondary poisoning)

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The degradation rate in water or air is  $t_{1/2} < 120$  min. Therefore, the substance potassium tert-butyrate itself is not likely to have any significant effect on sewage treatment systems. Instead, the effects profile of potassium tert-butyrate is determined by the hydrolysis product tert-butyl alcohol. The second hydrolysis product, potassium hydroxide, is abundantly present in the environment and therefore not considered relevant for this assessment. Tert-butyl alcohol concentrations are considered for non compartment specific effects.

Due to the low  $\log K_{ow}$  of 0.3 and measured bioconcentration factor  $BCF = 1.09$ , no bio-accumulation is expected for tert-butyl alcohol and consequently secondary poisoning via the food chain is of no concern.

#### 7.5.1 Toxicity to birds

It is unlikely that a secondary poisoning risk exists for tert-butyl alcohol, as tert-butyl alcohol is

- readily biodegradable, and
- has a low potential for bioaccumulation ( $BCF = 1.09$ ).

#### 7.5.2 Toxicity to mammals

This point is covered by data provided in section 5.

#### 7.5.3 Calculation of $PNEC_{oral}$ (secondary poisoning)

There is no concern for secondary poisoning and therefore no  $PNEC_{oral}$  (secondary poisoning) needs to be derived.

### 7.6 Conclusion on the environmental classification and labelling

No classification due to the environmental effects is necessary for potassium tert-butyrate or its degradation products. Please also refer to Chapter 3 for details on the classification and labelling of Potassium tert-butyrate according to Annex I to Directive 67/548/EEC.

## 8 PBT AND VPVB ASSESSMENT

### 8.1 Assessment of PBT/vPvB Properties – Comparison with the Criteria of Annex XIII

#### 8.1.1 Persistence Assessment

Potassium tert-butyrate and its degradation products potassium hydroxide and tert-butyl alcohol are readily biodegradable. Therefore potassium tert-butyrate cannot be regarded as persistent.

### 8.1.2 Bioaccumulation Assessment

Potassium tert-butyrate does not become bioavailable, as decomposition occurs before the substance is absorbed. Therefore, potassium tert-butyrate cannot be regarded as bio-accumulative. Upon contact with water potassium tert-butyrate decomposes to form potassium hydroxide and tert-butyl alcohol.

Further reaction of the decomposition product potassium hydroxide with water yields potassium ions and water. As potassium hydroxide is very reactive, there is no bio-accumulation. For the degradation product tert-butyl alcohol the partition coefficient is  $\log K_{ow} = 0.3$  and measured  $BCF = 1.09$ . Thus, the degradation product tert-butyl alcohol cannot be regarded as bio-accumulative.

### 8.1.3 Toxicity Assessment

Potassium tert-butyrate or its degradation products is not classified as toxic according to Annex I to 67/548/EEC and the data on toxicity provided herein.

### 8.1.4 Summary and overall Conclusions on PBT or vPvB Properties

Potassium tert-butyrate or its degradation products are no PBT or vPvB substances.

## 8.2 Emission Characterisation

Not needed as potassium tert-butyrate or its degradation products are neither PBT nor vPvB substances.

## 9 EXPOSURE ASSESSMENT

Table 14: Overview on exposure scenarios and coverage of substance life cycle

Exposure Scenario	Manufacture	Preparation making	Industrial and/or wide disperse use	Consumer use	Article service life	Waste stage
Use 0: Production	X	-	-	-	-	-
Use 1: Reagent in chemical synthesis	-	-	X	-	-	-

### 9.1 Use 0: Production of potassium tert-butylate

#### 9.1.1 Exposure scenario

##### *Description of process:*

Potassium tert-butylate is manufactured by adding Potassium to tert-butyl alcohol. Subsequently, Potassium tert-butylate is separated and cleaned by distillation. Production takes place in closed systems under inert gas atmosphere. Any cleaning solutions of production reaction vessels are incinerated.

A production volume of 50 tonnes / year is assumed for this CSR example.

The processes involved in the potassium tert-butylate production can be categorized by the descriptor system as follows:

According to the use descriptor system this use can be categorised as follows:

Sector of use: SU3 "Industrial Manufacturing"

Product category: Not relevant; the substance is not used in consumer products

Process categories: PROC1 "Used in closed processes, no likelihood of exposure; industrial setting"

PROC2 "Use in closed, continuous process with occasional controlled exposure (e.g. sampling); industrial setting"

Article category: Not relevant

Environmental release category: Not relevant; the substance decomposes spontaneously upon contact with water or air

#### 9.1.1.1 Risk management measures

##### 9.1.1.1.1 Risk management measures related to workers

All production processes are carried out in closed systems under inert gas atmosphere. Adequate personal protection equipment (gloves, goggles, and coverall, see SDS for details) is provided, automatic systems for sampling are used and workers are informed on potential risks.

**9.1.1.1.2**      Risk management measures related to environment

Do not allow to directly enter the environment.

Any potential releases to air or water should be avoided.

**9.1.1.1.3**      Waste related measures

Any wastes and cleaning solutions that can contain residues of potassium tert-butyrate are incinerated.

**9.1.2**      **Exposure estimation****9.1.2.1**      **Worker exposure**

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The degradation rate in water or air is  $t_{1/2} < 120$  min. Thus, there is practically no exposure of potassium tert-butyrate to workers. Potassium tert-butyrate is not bioavailable as decomposition occurs before absorption. Instead the decomposition products potassium hydroxide and tert-butyl alcohol need to be considered.

The hydrolysis product potassium hydroxide further reacts with tissues to produce potassium ions and water. Potassium is an essential element in human nutrition. Therefore, potassium hydroxide is not considered relevant for this exposure assessment.

Model calculations for potassium tert-butyrate and the decomposition product tert-butyl alcohol were performed using ECETOC TRA. The following table gives an overview on the scenarios assessed in relation to the process categories according to the descriptor system:

Table 15: ECETOC TRA scenarios (Use 0)

No.	Process category according to descriptor system	ECETOC TRA Exposure Scenario (non-dispersive uses)
1	PROC1 "Used in closed processes, no likelihood of exposure; industrial setting"	Use in a closed continuous process
2	PROC2 "Use in closed, continuous process with occasional controlled exposure (e.g. sampling); industrial setting"	Use in a continuous process (with process sampling)

Worker exposure process categories 1 and 2 (PROC1 and PROC2) only include inhalation exposure. The production processes considered do not include dermal exposure, as production takes place in closed systems only.

The following table summarises the ECETOC TRA output for potassium tert-butyrate inhalative exposure for scenarios PROC1 and PROC2.

Table 16: ECETOC TRA model calculations for potassium tert-butyrate (Use 0, inhalation)

Type	Scenario	Duration of Activity	Local exhaustive ventilation [Y/N]	Estimated Exposure [mg/m <sup>3</sup> ]
Non-dispersive	Closed continuous	> 4 hours	Yes	0.010
Non-dispersive	Continuous	> 4 hours	Yes	0.100

The following table summarises the ECETOC TRA output for tert-butyl alcohol inhalative exposure for scenarios PROC1 and PROC2.

Table 17: ECETOC TRA model calculations for potassium tert-butyrate (Use 0, inhalation)

Type	Scenario	Duration of Activity	Local exhaustive ventilation [Y/N]	Estimated Exposure [ppm / mg/m <sup>3</sup> ]
Non-dispersive	Closed continuous	> 4 hours	Yes	0.010/0.03
Non-dispersive	Continuous	> 4 hours	Yes	20.0/60.63

For potassium tert-butyrate and tert-butyl alcohol the ECETOC TRA model calculations estimated inhalation exposures of 0.01 mg/m<sup>3</sup> to 0.1 mg/m<sup>3</sup> and 0.01 ppm to 20.0 ppm (0.03 mg/m<sup>3</sup> to 60.63 mg/m<sup>3</sup>) for the different production and use scenarios. For both parent substance and decomposition product air concentrations are below the tert-butyl alcohol inhalation DNEL<sub>acute, inhal</sub> = 1,333 ppm (4042 mg/m<sup>3</sup>) and the DNEL<sub>long-term, inhal</sub> = 280 ppm (849 mg/m<sup>3</sup>).

#### 9.1.2.2 Indirect exposure of humans via the environment

Indirect exposure of humans to potassium tert-butyrate via the environment can be excluded, due to the reactive nature of the substance. The decomposition product potassium hydroxide is not considered relevant, as potassium hydroxide further reacts with water/(organic) acids to produce potassium ions and potassium is an abundant element in the environment. Further, there is no tendency for tert-butyl alcohol to bio-accumulate. Therefore, there is no risk of indirect exposure of humans.

#### 9.1.2.3 Environmental exposure

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The degradation rate in water or air is  $t_{1/2} < 120$  min. The reaction with water is violent (R14; reacts violently with water). Therefore, there is practically no exposure of potassium tert-butyrate to the aquatic environment. Instead the decomposition products potassium hydroxide and tert-butyl alcohol need to be considered.

The hydrolysis product potassium hydroxide further reacts with water to produce potassium ions and water. Potassium is the seventh most abundant element, present as various compounds, making up about 1.5% of the weight of the Earth's crust (Winter, 2008). Therefore, potassium hydroxide is not considered relevant for exposure assessment.

Environmental exposure to tert-butyl alcohol was assessed using EUSES 2.0.3 and is summarised in the tables below. For details please refer to the EUSES report in Appendix II.

Table 18: Duration, frequency and amounts related to emissions from production (Use 0)

Information type	Data field	Explanation
Annual amount used per site	50 tonnes/year	--
Emission days per site	292 days/year	This figure was set in the EUSES calculation overriding the default value, based on the assumption of an average utilisation of 80%. This figure is considered to represent a worst case scenario.
Other determinants related to duration, frequency and amount	The calculations assume that all potassium tert-butyrate is available as tert-butyl alcohol, i.e. 50 tonnes /year	This assumption is considered to represent a worst-case scenario.

The EUSES exposure calculations assume that all potassium tert-butyrate is available as tert-butyl alcohol i.e. 50 tonnes /year.

Table 19: Use 0 – Tert-butyl alcohol Predicted Exposure Concentrations (PECs)

Compartments	Local concentration single instance / continuous	PEC <sup>1</sup> (local+regional)	Justification
Surface water (in mg/L)	7.15 / 5.72		--
Fresh water sediment (in mg/kgwwt)	7.93 / --		--
Sea water (mg/L)	0.774 / 0.619		--
Marine sediment (mg/kgwwt)	0.858 / --		--
Agricultural soil total (mg/kgwwt)	0.467 (30 d average)		--
STP (mg/L)	71.5 /--		
Groundwater (mg/L)	0.637 (180 d average)		--
Grassland total (mg/kgwwt)	0.0567 (180 d average)		--
Air (mg/m <sup>3</sup> )	4.56E-03 / 3.65E-03		--

<sup>1</sup> Regional PECs are negligible compared to local PECs (see EUSES report). Therefore, no summation of local and regional PECs was performed.

Concentrations of tert-butyl alcohol were determined in water, sediment and air for single instances and continuous exposure. Highest concentrations in the aquatic compartment were determined for single instance exposures to surface water (7.15 mg/L).

## 9.2 Use 1: Reagent in chemical synthesis

### 9.2.1 Exposure scenario

#### *Description of process:*

Potassium tert-butyrate is used in closed systems under inert gas atmosphere only. During the reaction process the substance is completely converted chemically. Any cleaning solutions of reaction vessels are incinerated.

According to the use descriptor system this use can be categorised as follows:



Sector of use:	SU3 "Industrial Manufacturing"
Product category:	Not relevant; the substance is not used in consumer products
Process categories:	PROC1 "Used in closed processes, no likelihood of exposure; industrial setting"  PROC2 "Use in closed, continuous process with occasional controlled exposure (e.g. sampling); industrial setting"  PROC3 "Use in closed continuous batch process (synthesis); industrial setting"  PROC4 "Use in a batch or other process (including related process stages e.g. filtration, drying) where opportunities for exposure arise (synthesis); industrial setting"
Article category:	Not relevant
Environmental release category:	Not relevant; the substance decomposes spontaneously upon contact with water or air

#### **9.2.1.1 Risk management measures**

##### **9.2.1.1.1 Risk management measures related to workers**

All production processes are carried out in closed systems under inert gas atmosphere. Adequate personal protection equipment (gloves, goggles, and coverall, see SDS for details) is provided, automatic systems for sampling are used and workers are informed on potential risks.

##### **9.2.1.1.2 Risk management measures related to environment**

Do not allow to directly enter the environment.

Any potential releases to air or water should be avoided.

##### **9.2.1.1.3 Waste related measures**

Any wastes and cleaning solutions that can contain residues of potassium tert-butyrate are incinerated.

#### **9.2.2 Exposure estimation**

##### **9.2.2.1 Worker exposure**

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The degradation rate in water or air is  $t_{1/2} < 120$  min. Thus, there is practically no exposure of potassium tert-butyrate to workers. Potassium tert-butyrate is not bioavailable as decomposition occurs before absorption. Instead the decomposition products potassium hydroxide and tert-butyl alcohol need to be considered.

The hydrolysis product potassium hydroxide further reacts to produce potassium ions and water. Potassium is an essential element in human nutrition. Therefore, potassium hydroxide is not considered relevant for this exposure assessment.

Model calculations for potassium tert-butyrate and the decomposition product tert-butyl alcohol were performed using ECETOC TRA. The following table gives an overview on the scenarios assessed in relation to the process categories according to the descriptor system:

Table 20: ECETOC TRA scenarios (Use 1)

No.	Process category according to descriptor system	ECETOC TRA exposure scenarios (non-dispersive uses)
1	PROC1 "Used in closed processes, no likelihood of exposure; industrial setting"	Use in a closed continuous process
2	PROC2 "Use in closed, continuous process with occasional controlled exposure (e.g. sampling); industrial setting"	Use in a continuous process (with process sampling)
3	PROC3 "Use in closed continuous batch process (synthesis); industrial setting"	Batch manufacture of a chemical or formulation where the predominant handling is in a contained manner
4	PROC4 "Use in a batch or other process (including related process stages e.g. filtration, drying) where opportunities for exposure arise (synthesis); industrial setting"	Use in the batch manufacture of a chemical where significant opportunity for exposure arises e.g. during the charging, sampling or discharge of materials, and when the nature of the design can reasonably be predicted to result in exposures

The following table summarises the ECETOC TRA output for potassium tert-butyrate inhalative exposure for the scenarios listed above (Use 1).

Table 21: ECETOC TRA model calculations for potassium tert-butyrate (Use 1, inhalation)

Type	Scenario	Duration of Activity	Local exhaustive ventilation [Y/N]	Estimated Exposure [mg/m <sup>3</sup> ]
Non-dispersive	Closed continuous	> 4 hours	Yes	0.01
Non-dispersive	Continuous	> 4 hours	Yes	0.1
Non-dispersive	Closed batch	> 4 hours	Yes	0.1
Non-dispersive	Mixing, blending or calendering	> 4 hours	Yes	0.5

The following table summarises the ECETOC TRA output for tert-butyl alcohol inhalative exposure for the scenarios listed above (Use 1).

Table 22: ECETOC TRA model calculations for potassium tert-butyl alcohol (Use 1, inhalation)

Type	Scenario	Duration of Activity	Local exhaustive ventilation [Y/N]	Estimated Exposure [ppm / mg/m <sup>3</sup> ]
Non-dispersive	Closed continuous	> 4 hours	Yes	0.010/0.03
Non-dispersive	Continuous	> 4 hours	Yes	20.00/60.63
Non-dispersive	Closed batch	> 4 hours	Yes	20.00/60.63
Non-dispersive	Mixing, blending or calendering	> 4 hours	Yes	100.00/303.16

The model calculations for inhalation exposure show estimated exposures of 0.01 mg to 0.5 mg and 0.01 to 100 ppm (0.003 to 303 mg/m<sup>3</sup>) for potassium tert-butyrate and tert-butyl alcohol, respectively. The concentrations in air are below the tert-butyl alcohol DNEL<sub>acute, inhal</sub> = 1,333 ppm (4042 mg/m<sup>3</sup>) and the DNEL<sub>long-term, inhal</sub> = 280 ppm (849 mg/m<sup>3</sup>).

The following table summarises the ECETOC TRA output for potassium tert-butyrate dermal exposure for the scenarios listed above (Use 1).

Table 23: ECETOC TRA model calculations for potassium tert-butyrate (Use 1, dermal)

Type	Scenario	Duration of Activity	Local exhaustive ventilation [Y/N]	Estimated Exposure [mg/kg bw/day]
On-site uses	Batch or other	> 4 hours	Yes	0.07
Non-dispersive	Mixing, blending or calendering	> 4 hours	Yes	0.07

The following table summarises the ECETOC TRA output for tert-butyl alcohol dermal exposure for the scenarios listed above (Use 1).

Table 24: ECETOC TRA model calculations for potassium tert-butyl alcohol (Use 1, dermal)

Type	Scenario	Duration of Activity	Local exhaustive ventilation [Y/N]	Estimated Exposure [mg/kg bw/day]
On-site uses	Batch or other	> 4 hours	Yes	0.07
Non-dispersive	Mixing, blending or calendering	> 4 hours	Yes	0.07

The model calculations for dermal exposure for both substances, potassium tert-butyrate and tert-butyl alcohol, show an estimated exposure of 0.07 mg/kg bw/day for the described process category affected (PROC4). The estimated dermal concentrations are below the tert-butyl alcohol dermal DNEL<sub>acute, dermal</sub> of 34.5 mg/kg bw and DNEL<sub>long-term, dermal</sub> = 11.72 mg/kg bw/day.

### 9.2.2.2 Indirect exposure of humans via the environment

Indirect exposure of humans to potassium tert-butyrate via the environment can be excluded, due to the reactive nature of the substance. The decomposition product potassium hydroxide is not considered relevant, as potassium hydroxide further reacts with water/(organic) acids to produce potassium ions and potassium is an abundant element in the environment. Further, there is no tendency for tert-butyl alcohol to bio-accumulate. Therefore, there is no risk of indirect exposure of humans.

### 9.2.2.3 Environmental exposure

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The degradation rate in water or air is  $t_{1/2} < 120$  min. The reaction with water is violent (R14; reacts violently with water). Therefore, there is practically no exposure of potassium tert-butyrate to the aquatic environment. Instead the decomposition products potassium hydroxide and tert-butyl alcohol need to be considered.

The hydrolysis product potassium hydroxide further reacts with water/(organic) acids to produce potassium ions and water. Potassium is the seventh most abundant element, present as various compounds, making up about 1.5% of the weight of the Earth's crust (Winter, 2008). Therefore, potassium hydroxide is not considered relevant for exposure assessment.

Environmental exposure to tert-butyl alcohol was assessed using EUSES 2.0.3 and is summarised in the tables below. For details please refer to the EUSES report in Appendix II.

Table 25: Duration, frequency and amounts related to emissions from production (Use 1)

Information type	Data field	Explanation
Annual amount used per site	50 tonnes/year	--
Emission days per site	292 days/year	This figure was set in the EUSES calculation overriding the default value, based on the assumption of an average utilisation of 80%. This figure is considered to represent a worst case scenario.
Other determinants related to duration, frequency and amount	The calculations assume that all potassium tert-butyrate is available as tert-butyl alcohol, i.e. 50 tonnes /year	This assumption is considered to represent a worst-case scenario.

The EUSES exposure calculations assume that all potassium tert-butyrate is available as tert-butyl alcohol i.e. 50 tonnes /year.

Table 26: Use 1 – Tert-butyl alcohol Predicted Exposure Concentrations (PECs)

Compartments	Local concentration single instance / continuous	PEC <sup>1</sup> (local+regional)	Justification
Surface water (in mg/L)	2.31 / 0.0633		--
Fresh water sediment (in mg/kgwwt)	2.56 / --		--
Sea water (mg/L)	0.25 / 6.85E-03		--
Marine sediment (mg/kgwwt)	0.277 / --		--
Agricultural soil total (mg/kgwwt)	0.15 (30 d average)		--
STP (mg/L)	23.1 / --		
Groundwater (mg/L)	0.204 / (180 d average)		--
Grassland total (averaged over 180 days; mg/kgwwt)	0.0177 (180 d average)		--
Air (mg/m <sup>3</sup> )	0.0174 / 4.76E-04		--

<sup>1</sup> Regional PECs are negligible compared to local PECs (see EUSES report). Therefore, no summation of local and regional PECs was performed.

Concentrations of tert-butyl alcohol were determined in water, sediment and air for single instances and continuous exposure. Highest concentrations in the aquatic compartment were determined for single instance exposures to surface water (2.31 mg/L).

### 9.3 Regional and continental exposure concentrations

Regional exposure concentrations are negligible and therefore not considered further. Please refer to the EUSES report in Appendix II for details.

## 10 RISK CHARACTERISATION

### 10.1 Use 0: Production of Potassium tert-butylate

#### 10.1.1 Human health

##### 10.1.1.1 Risk Characterisation for Workers

Potassium tert-butylate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The degradation rate in water or air is  $t_{1/2} < 120$  min. Thus, there is practically no exposure of potassium tert-butylate to workers. Potassium tert-butylate is not bioavailable as decomposition occurs before absorption. Instead the decomposition products potassium hydroxide and tert-butyl alcohol need to be considered.

The hydrolysis product potassium hydroxide further reacts to produce potassium ions and water. Potassium is an essential element in human nutrition. Therefore, potassium hydroxide is not considered relevant for this exposure assessment.

Model calculations for potassium tert-butylate and the decomposition product tert-butyl alcohol were performed using ECETOC TRA. Potassium tert-butylate DNELs were derived on the basis of systemic toxicity, which is determined by its degradation product tert-butyl alcohol. The following

risk characterisation covers the full range of possible exposures to either the parent compound or its degradation product for acute and long-term periods.

The following table shows risk characterisations for the full range of exposure values of both, potassium tert-butyrate and degradation product tert-butyl alcohol.

Table 27: Quantitative risk characterisation for workers based on modelled data

UEC Matrix Element	Process Categories	Estimated Exposure [ppm]	LEV	Duration of activity	DNEL Inhalation [ppm]	Risk characterisation ratio
13 Inhalation Short-term	PROC1	0.010 (low range)	yes	> 4 hours	1,333	7.50E-06
	PROC2	20.0 (high range)	yes	> 4 hours	1,333	0.015
16 Inhalation Long-term/ repeated	PROC1	0.010 (low range)	yes	> 4 hours	280	3.57E-05
	PROC2	20.0 (high range)	yes	> 4 hours	280	0.071

For Use 0 the risk for the human health (workers) is considered to be acceptable for all relevant process categories, as all risk characterisation ratios (exposure/DNEL) values are below the trigger value of one.

*Conclusion (i):* the substance is of no immediate concern for man.

### 10.1.1.2 Indirect exposure of humans via the environment

Not relevant, see chapter 9.1.2.2.

## 10.1.2 Environment

### 10.1.2.1 Risk Characterisation (PEC/PNEC)

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The degradation rate in water or air is  $t_{1/2} < 120$  min. The reaction with water is violent (R14; reacts violently with water). Therefore, there is practically no exposure of potassium tert-butyrate to the aquatic environment. Instead the decomposition products potassium hydroxide and tert-butyl alcohol need to be considered.

The hydrolysis product potassium hydroxide further reacts with water/(organic) acids to produce potassium ions and water. Potassium is the seventh most abundant element, present as various compounds, making up about 1.5% of the weight of the Earth's crust (Winter, 2008). Therefore, potassium hydroxide is not considered relevant for exposure assessment.

The table below shows the quantitative risk characterisation for the different environmental compartments based on tert-butyl alcohol PEC and PNEC derivation. The compartments shown represent the worst case scenarios for single instance and continuous exposure.

Table 28: Quantitative risk characterisation for environmental compartments

UEC Matrix Element	Compartments	Local PEC single instance / continuous	PNEC	PEC/PNEC single instance / continuous
19 Environment: Water, Short-term / 22 Environment: Water, Continuous	Surface water (mg/L)	7.15 / 5.72	9.3	0.7688 / 0.6151
	Fresh water sediment (mg/kgwwt)	7.93 / --	10.3	0.7699 / --
	Sea water (mg/L)	0.774 / 0.619	0.93	0.8323 / 0.6656
	Marine sediment (mg/kgwwt)	0.858 / --	1.03	0.8330 / --
	Agricultural soil total (mg/kgwwt)	0.467 (30 d average)	16.4	0.0285
	STP (mg/L)	71.5 / --	1,000	0.0715 / --
25 Environment: Air, Short-term / 28 Environment: Air, continuous	Air (mg/m <sup>3</sup> )	4.56E-03 / 3.65E-03	1,333 (DNEL <sub>short-term, inhal</sub> ) 280 (DNEL <sub>long-term, inhal</sub> )	3.42E-06 / 1.30E-05

The risk for the environment is considered to be acceptable for all relevant compartments for single instance and continuous exposure. All PEC/PNEC values are below the trigger value of one.

*Conclusion (i):* the substance is of no immediate concern for the environment.

## 10.2 Use 1: Reagent in chemical synthesis

### 10.2.1 Human health

#### 10.2.1.1 Risk Characterisation for workers

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The degradation rate in water or air is  $t_{1/2} < 120$  min. Thus, there is practically no exposure of potassium tert-butyrate to workers. Potassium tert-butyrate is not bioavailable as decomposition occurs before absorption. Instead the decomposition products potassium hydroxide and tert-butyl alcohol need to be considered.

The hydrolysis product potassium hydroxide further reacts to produce potassium ions and water. Potassium is an essential element in human nutrition. Therefore, potassium hydroxide is not considered relevant for this exposure assessment.

Model calculations for potassium tert-butyrate and the decomposition product tert-butyl alcohol were performed using ECETOC TRA. Potassium tert-butyrate DNELs were derived on the basis of systemic toxicity, which is determined by its degradation product tert-butyl alcohol. The following risk characterisation covers the full range of possible exposures to either the parent compound or its degradation product for acute and long-term periods.

The following table shows risk characterisations for the full range of exposure values of both, potassium tert-butyrate and degradation product tert-butyl alcohol.

Table 29: Quantitative risk characterisation for workers based on modelled data in terms of generic exposure scenarios\*

UEC Matrix Element	Process Categories	Estimated Exposure [mg/kg bw/day]	LEV	Duration of activity	DNEL Dermal [mg/kg bw/day] Inhalation [ppm]	Risk characterisation ratio
7 Dermal Short-term	PROC4	0.07	yes	> 4 hours	34.5	0.002
10 Dermal Long-term/ repeated	PROC4	0.07	yes	> 4 hours	11.72	0.006
13 Inhalation Short-term	PROC1 PROC2 PROC3 PROC4	0.010 (low range) 20.0 20.0 100.0 (high range)	yes yes yes yes	> 4 hours > 4 hours > 4 hours > 4 hours	1,333 1,333 1,333 1,333	7.50E-06 0.015 0.015 0.075
16 Inhalation Long-term/ repeated	PROC1 PROC2 PROC3 PROC4	0.010 20.0 20.0 100.0	yes yes yes yes	> 4 hours > 4 hours > 4 hours > 4 hours	280 280 280 280	3.57E-05 0.071 0.071 0.48

\*Dermal risk characterisation does not take corrosive properties of the substance into account.

The above risk characterisation does not account for the corrosive properties of Potassium tert-butylate or potassium hydroxide. Workers need to follow RMM to ensure that no dermal corrosion occurs.

For Use 1 the risk for the human health (workers) is considered to be acceptable for all relevant process categories (PROC1 to PROC4), as all risk characterisation ratios (exposure/DNEL) values are below the trigger value of one.

*Conclusion (i):* the substance is of no immediate concern for man.

#### 10.2.1.2 Indirect exposure of humans via the environment

Not relevant, see chapter 9.2.2.2



## 10.2.2 Environment

### 10.2.2.1 Risk Characterisation (PEC/PNEC)

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The degradation rate in water or air is  $t_{1/2} < 120$  min. The reaction with water is violent (R14; reacts violently with water). Therefore, there is practically no exposure of potassium tert-butyrate to the aquatic environment. Instead the decomposition products potassium hydroxide and tert-butyl alcohol need to be considered.

The hydrolysis product potassium hydroxide further reacts with water/(organic) acids to produce potassium ions and water. Potassium is the seventh most abundant element, present as various compounds, making up about 1.5% of the weight of the Earth's crust (Winter, 2008). Therefore, potassium hydroxide is not considered relevant for exposure assessment.

The table below shows the quantitative risk characterisation for the different environmental compartments based on tert-amyl alcohol PEC and PNEC derivation. The compartments shown represent the worst case scenarios for single instance and continuous exposure.

Table 30: Quantitative risk characterisation for environmental compartments

UEC Matrix Element	Compartments	Local PEC single instance / continuous	PNEC	PEC/PNEC single instance / continuous
19 Environment: Water, Short-term / 22 Environment: Water, Continuous	Surface water (mg/L)	2.31 / 0.0633	9.3	0.2484 / 6.81E-03
	Fresh water sediment (mg/kgwwt)	2.56 / --	10.3	0.2485 / --
	Sea water (mg/L)	0.25 / 6.85E-03	0.93	0.2688 / 7.37E-03
	Marine sediment (mg/kgwwt)	0.277 / --	1.03	0.2689 / --
	Agricultural soil total (mg/kgwwt)	0.15 (30 d average)	16.4	0.0091
	STP (mg/L)	23.1 / --	1,000	0.0231 / --
25 Environment: Air, Short-term / 28 Environment: Air, continuous	Air (mg/m <sup>3</sup> )	0.0174 / 4.76E-04	1,333 (DNEL <sub>short-term inhal</sub> ) 280 (DNEL <sub>long-term inhal</sub> )	1.30E-05 / 1.70E-06

The risk for the environment is considered to be acceptable for all relevant compartments for single instance and continuous exposure. All PEC/PNEC values are below the trigger value of one.

*Conclusion (i):* the substance is of no immediate concern for the environment.

## 10.3 Overall exposure (combined for all relevant emission/release sources)

### 10.3.1 Human health (combined for all exposure routes)

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The degradation rate in water or air is  $t_{1/2} < 120$  min. Thus, there is practically no exposure of potassium tert-butyrate to workers. Potassium tert-butyrate is not

bioavailable as decomposition occurs before absorption. Instead the decomposition products potassium hydroxide and tert-butyl alcohol need to be considered.

The hydrolysis product potassium hydroxide further reacts to produce potassium ions and water. Potassium is an essential element in human nutrition. Therefore, potassium hydroxide is not considered relevant for the overall risk assessment.

Model calculations for potassium tert-butyrate and the decomposition product tert-butyl alcohol were performed. Potassium tert-butyrate DNELs were derived on the basis of systemic toxicity, which is determined by its degradation product tert-butyl alcohol. Acute and long-term exposures were considered. The production plant work pattern and work patterns of industries using potassium tert-butyrate as reagent in chemical synthesis are similar. Finally, there is practically no indirect exposure of the substance to humans. Thus, worker exposure to more than one source of potassium tert-butyrate does practically not occur.

*Conclusion (i):* the substance is of no immediate concern for man.

### 10.3.2 Environment (combined for all emission sources)

Potassium tert-butyrate reacts spontaneously with water (and water vapour) to form tert-butyl alcohol and potassium hydroxide. The degradation rate in water or air is  $t_{1/2} < 120$  min. The reaction with water is violent (R14; reacts violently with water). Therefore, there is practically no exposure of potassium tert-butyrate to the aquatic environment. Instead the decomposition products potassium hydroxide and tert-butyl alcohol need to be considered.

The hydrolysis product potassium hydroxide further reacts with water/(organic) acids to produce potassium ions and water. Potassium is the seventh most abundant element, present as various compounds, making up about 1.5% of the weight of the Earth's crust (Winter, 2008). Therefore, potassium hydroxide is not considered relevant for the overall risk assessment.

Local predicted environmental concentrations are highest and regional as well as continental concentrations are negligible. Thus, environmental exposure to more than one source of potassium tert-butyrate does practically not occur.

*Conclusion (i):* the substance is of no immediate concern for man.

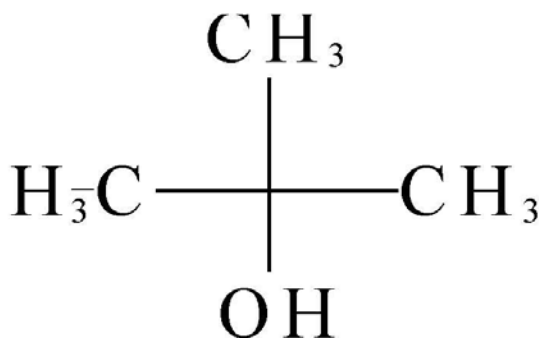
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IUCLID Dataset Tert-Butyl Alcohol (2000)

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**Appendix I:****Tert-butyl  
alcohol****EpiWin (v3.12)**

SMILES : CC(C)(C)O  
 CHEM :  
 MOL FOR: C4 H10 O1  
 MOL WT : 74.12

----- EPI SUMMARY (v3.12) -----  
 Physical Property Inputs:  
 Water Solubility (mg/L): -----  
 Vapor Pressure (mm Hg): -----  
 Henry LC (atm-m3/mole): -----  
 Log Kow (octanol-water): -----  
 Boiling Point (deg C) : -----  
 Melting Point (deg C) : -----

**KOWWIN Program (v1.67) Results:**

=====

Log Kow(version 1.67 estimate): 0.73

SMILES : CC(C)(C)O  
 CHEM :  
 MOL FOR: C4 H10 O1  
 MOL WT : 74.12

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	-CH3 [aliphatic carbon]	0.5473	1.6419
Frag	1	-OH [hydroxy, aliphatic attach]	-1.4086	-1.4086
Frag	1	-tert Carbon [3 or more carbon attach]	0.2676	0.2676
Const		Equation Constant		0.2290
Log Kow =				0.7299

**MPBPWIN (v1.41) Program Results:**

=====

SMILES : CC(C)(C)O  
 CHEM :  
 MOL FOR: C4 H10 O1  
 MOL WT : 74.12

----- SUMMARY MPBPWIN v1.41 -----

Boiling Point: 70.42 deg C (Adapted Stein and Brown Method)

Melting Point: -75.08 deg C (Adapted Joback Method)

Melting Point: -72.55 deg C (Gold and Ogle Method)

Mean Melt Pt : -73.81 deg C (Joback; Gold, Ogle Methods)

Selected MP: -73.81 deg C (Mean Value)

**Vapor Pressure Estimations (25 deg C):**

(Using BP: 70.42 deg C (estimated))

(MP not used for liquids)

VP: 92.1 mm Hg (Antoine Method)

VP: 87 mm Hg (Modified Grain Method)

VP: 146 mm Hg (Mackay Method)

Selected VP: 89.6 mm Hg (Mean of Antoine &amp; Grain methods)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	3	-CH3	21.98	65.94
Group	1	>C<	4.50	4.50
Group	1	-OH (tertiary)	69.32	69.32
*		Equation Constant		198.18
=====				
RESULT-uncorr		BOILING POINT in deg Kelvin		337.94
RESULT- corr		BOILING POINT in deg Kelvin		343.58
		BOILING POINT in deg C		70.42

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	3	-CH3	-5.10	-15.30
Group	1	>C<	46.43	46.43
Group	1	-OH (tertiary)	44.45	44.45
*		Equation Constant		122.50
=====				
RESULT		MELTING POINT in deg Kelvin		198.08
		MELTING POINT in deg C		-75.08

Water Sol from Kow (WSKOW v1.41) Results:

=====

Water Sol: 1.03e+005 mg/L

SMILES : CC(C)(C)O

CHEM :

MOL FOR: C4 H10 O1

MOL WT : 74.12

----- WSKOW v1.41 Results -----

Log Kow (estimated) : 0.73

Log Kow (experimental): not available from database

Log Kow used by Water solubility estimates: 0.73

Equation Used to Make Water Sol estimate:

Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction  
(used when Melting Point NOT available)

Correction(s): Value

-----

Alcohol, aliphatic 0.510

Log Water Solubility (in moles/L) : 0.143

Water Solubility at 25 deg C (mg/L): 1.03e+005

WATERNT Program (v1.01) Results:

=====

Water Sol (v1.01 est): 1.511e+005 mg/L

SMILES : CC(C)(C)O

CHEM :

MOL FOR: C4 H10 O1

MOL WT : 74.12

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	-CH3 [aliphatic carbon]	-0.3213	-0.9638
Frag	1	-OH [hydroxy, aliphatic attach]	1.6012	1.6012
Frag	1	-tert Carbon [3 or more carbon attach]	-0.5774	-0.5774
Const		Equation Constant		0.2492

Log Water Sol (moles/L) at 25 dec C = 0.3093

Water Solubility (mg/L) at 25 dec C =1.511e+005

ECOSAR Program (v0.99h) Results:

=====

SMILES : CC(C)(C)O  
 CHEM :  
 CAS Num:  
 ChemID1:  
 ChemID2:  
 ChemID3:  
 MOL FOR: C4 H10 O1  
 MOL WT : 74.12  
 Log Kow: 0.73 (KowWin estimate)  
 Melt Pt:  
 Wat Sol: 6507 mg/L (calculated)

ECOSAR v0.99h Class(es) Found

-----

Neutral Organics

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
=====	=====	=====	=====	=====
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	1270.948
Neutral Organics	: Fish	96-hr	LC50	858.534
Neutral Organics	: Fish	14-day	LC50	1270.948
Neutral Organics	: Daphnid	48-hr	LC50	842.670
Neutral Organics	: Green Algae	96-hr	EC50	489.675
Neutral Organics	: Fish	30-day	ChV	90.128
Neutral Organics	: Daphnid	16-day	EC50	24.795
Neutral Organics	: Green Algae	96-hr	ChV	23.504
Neutral Organics	: Fish (SW)	96-hr	LC50	106.428
Neutral Organics	: Mysid Shrimp	96-hr	LC50	612.996
				mg/kg (ppm) dry wt soil
				=====
Neutral Organics	: Earthworm	14-day	LC50	1122.323

Note: \* = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.  
 Fish and daphnid acute toxicity log Kow cutoff: 5.0  
 Green algal EC50 toxicity log Kow cutoff: 6.4  
 Chronic toxicity log Kow cutoff: 8.0  
 MW cutoff: 1000

HENRY (v3.10) Program Results:

=====

Bond Est : 9.99E-006 atm-m3/mole  
 Group Est: 1.04E-005 atm-m3/mole

SMILES : CC(C)(C)O  
 CHEM :  
 MOL FOR: C4 H10 O1  
 MOL WT : 74.12

----- HENRYWIN v3.10 Results -----

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
+	+	+	+
HYDROGEN	9 Hydrogen to Carbon (aliphatic) Bonds		-1.0771
HYDROGEN	1 Hydrogen to Oxygen Bonds		3.2318
FRAGMENT	3 C-C		0.3489
FRAGMENT	1 C-O		1.0855
FACTOR	* Non-cyclic alkyl or olefinic alcohol		-.2000



RESULT	BOND ESTIMATION METHOD for LWAPC VALUE	TOTAL	3.389
--------	--	-------	-------

HENRYs LAW CONSTANT at 25 deg C = 9.99E-006 atm-m3/mole  
= 4.08E-004 unitless

	GROUP CONTRIBUTION DESCRIPTION	COMMENT	VALUE
3	CH3 (X)		-1.86
1	C (C) (C) (C) (O)		0.78
1	O-H (C)		4.45

RESULT	GROUP ESTIMATION METHOD for LOG GAMMA VALUE	TOTAL	3.37
--------	---	-------	------

HENRYs LAW CONSTANT at 25 deg C = 1.04E-005 atm-m3/mole  
= 4.27E-004 unitless

Henrys LC [VP/WSol estimate using EPI values]:

HLC: 8.484E-005 atm-m3/mole

VP: 89.6 mm Hg

WS: 1.03E+005 mg/L

BIOWIN (v4.02) Program Results:

SMILES : CC(C)(C)O

CHEM :

MOL FOR: C4 H10 O1

MOL WT : 74.12

----- BIOWIN v4.02 Results -----

Biowin1 (Linear Model Prediction) : Biodegrades Fast  
Biowin2 (Non-Linear Model Prediction): Biodegrades Fast  
Biowin3 (Ultimate Biodegradation Timeframe): Weeks  
Biowin4 (Primary Biodegradation Timeframe): Days-Weeks  
Biowin5 (MITI Linear Model Prediction) : Biodegrades Fast  
Biowin6 (MITI Non-Linear Model Prediction): Biodegrades Fast  
Ready Biodegradability Prediction: YES

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.1839	-0.1839
MolWt	*	Molecular Weight Parameter		-0.0353
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		0.5283

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Carbon with 4 single bonds & no hydrogens	-1.7232	-1.7232
MolWt	*	Molecular Weight Parameter		-1.0526
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.5580

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast  
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.2121	-0.2121
MolWt	*	Molecular Weight Parameter		-0.1638
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		2.8232

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.1534	-0.1534
MolWt	*	Molecular Weight Parameter		-0.1069
Const	*	Equation Constant		3.8477
RESULT		Biowin4 (Survey Model - Primary Biodeg)		3.5874

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks  
 (Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Carbon with 4 single bonds & no hydrogens	0.0676	0.0676
Frag	3	Methyl [-CH3]	0.0004	0.0012
MolWt	*	Molecular Weight Parameter		-0.2205
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.5605

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Carbon with 4 single bonds & no hydrogens	0.3990	0.3990
Frag	3	Methyl [-CH3]	0.0194	0.0583
MolWt	*	Molecular Weight Parameter		-2.1399
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.6991

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast  
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

## AOP Program (v1.91) Results:

SMILES : CC(C)(C)O  
 CHEM :  
 MOL FOR: C4 H10 O1  
 MOL WT : 74.12

----- SUMMARY (AOP v1.91): HYDROXYL RADICALS -----  
 Hydrogen Abstraction = 1.5504 E-12 cm3/molecule-sec  
 Reaction with N, S and -OH = 0.1400 E-12 cm3/molecule-sec  
 Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec  
 Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec  
 Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec  
 Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 1.6904 E-12 cm3/molecule-sec  
 HALF-LIFE = 6.327 Days (12-hr day; 1.5E6 OH/cm3)  
 HALF-LIFE = 75.930 Hrs

----- SUMMARY (AOP v1.91): OZONE REACTION -----

\*\*\*\*\* NO OZONE REACTION ESTIMATION \*\*\*\*\*  
 (ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NOT Available

## PCKOC Program (v1.66) Results:

Koc (estimated): 1.47



SMILES : CC(C)(C)O  
 CHEM :  
 MOL FOR: C4 H10 O1  
 MOL WT : 74.12

----- PCKOCWIN v1.66 Results -----  
 First Order Molecular Connectivity Index ..... : 2.000  
 Non-Corrected Log Koc ..... : 1.6870  
 Fragment Correction(s):  
     1 Aliphatic Alcohol (-C-OH) ..... : -1.5193  
 Corrected Log Koc ..... : 0.1677  
  
 Estimated Koc: 1.471

HYDROWIN Program (v1.67) Results:

=====

SMILES : CC(C)(C)O  
 CHEM :  
 MOL FOR: C4 H10 O1  
 MOL WT : 74.12

----- HYDROWIN v1.67 Results -----  
  
 Currently, this program can NOT estimate a hydrolysis rate constant for  
     the type of chemical structure entered!!  
  
 ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens)  
     and Specific Alkyl Halides can be estimated!! For more information,  
     (click OVERVIEW in Help or see the User's Guide)  
  
 \*\*\*\*\* CALCULATION NOT PERFORMED \*\*\*\*\*

BCF Program (v2.15) Results:

=====

SMILES : CC(C)(C)O  
 CHEM :  
 MOL FOR: C4 H10 O1  
 MOL WT : 74.12

----- Bcfwin v2.15 -----  
 Log Kow (estimated) : 0.73  
 Log Kow (experimental): not available from database  
 Log Kow used by BCF estimates: 0.73  
  
 Equation Used to Make BCF estimate:  
     Log BCF = 0.50  
  
     Correction(s):                      Value  
     Correction Factors Not Used for Log Kow < 1  
  
 Estimated Log BCF = 0.500 (BCF = 3.162)

Volatilization From Water  
 =====

Chemical Name:

Molecular Weight : 74.12 g/mole  
 Water Solubility : -----  
 Vapor Pressure : -----  
 Henry's Law Constant: 9.99E-006 atm-m3/mole (estimated by Bond SAR Method)

		RIVER	LAKE
		-----	-----
Water Depth	(meters):	1	1
Wind Velocity	(m/sec):	5	0.5

Current Velocity (m/sec): 1 0.05  
 HALF-LIFE (hours) : 51.33 632.2  
 HALF-LIFE (days ) : 2.139 26.34

# STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility

(using 10000 hr Bio P,A,S)

## PROPERTIES OF:

Molecular weight (g/mol)	74.12
Aqueous solubility (mg/l)	0
Vapour pressure (Pa)	0
(atm)	0
(mm Hg)	0
Henry 's law constant (Atm-m3/mol)	9.99E-006
Air-water partition coefficient	0.000408561
Octanol-water partition coefficient (Kow)	5.37032
Log Kow	0.73
Biomass to water partition coefficient	1.87406
Temperature [deg C]	25
Biodeg rate constants (h <sup>-1</sup> ), half life in biomass (h) and in 2000 mg/L MLSS (h):	
-Primary tank	0.02 37.34 10000.00
-Aeration tank	0.02 37.34 10000.00
-Settling tank	0.02 37.34 10000.00

## STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	1.3E-001	100.00
Primary sludge	2.62E-002	3.5E-004	0.26
Waste sludge	1.50E-001	2.0E-003	1.50
Primary volatilization	5.23E-003	7.1E-005	0.05
Settling volatilization	1.42E-002	1.9E-004	0.14
Aeration off gas	3.64E-002	4.9E-004	0.36
Primary biodegradation	1.76E-003	2.4E-005	0.02
Settling biodegradation	5.25E-004	7.1E-006	0.01
Aeration biodegradation	6.91E-003	9.3E-005	0.07
Final water effluent	9.76E+000	1.3E-001	97.58
Total removal	2.42E-001	3.3E-003	2.42
Total biodegradation	9.20E-003	1.2E-004	0.09

# STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility

(using Biowin/EPA draft method)

## PROPERTIES OF:

Molecular weight (g/mol)	74.12
Aqueous solubility (mg/l)	0
Vapour pressure (Pa)	0
(atm)	0
(mm Hg)	0
Henry 's law constant (Atm-m3/mol)	9.99E-006
Air-water partition coefficient	0.000408561
Octanol-water partition coefficient (Kow)	5.37032
Log Kow	0.73
Biomass to water partition coefficient	1.87406
Temperature [deg C]	25
Biodeg rate constants (h <sup>-1</sup> ), half life in biomass (h) and in 2000 mg/L MLSS (h):	
-Primary tank	18.56 0.04 10.00
-Aeration tank	185.59 0.00 1.00
-Settling tank	185.59 0.00 1.00

## STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	1.3E-001	100.00
Primary sludge	2.23E-002	3.0E-004	0.22
Waste sludge	1.22E-002	1.6E-004	0.12
Primary volatilization	4.45E-003	6.0E-005	0.04
Settling volatilization	1.15E-003	1.6E-005	0.01
Aeration off gas	3.81E-003	5.1E-005	0.04
Primary biodegradation	1.50E+000	2.0E-002	14.97
Settling biodegradation	4.25E-001	5.7E-003	4.25
Aeration biodegradation	7.24E+000	9.8E-002	72.43
Final water effluent	7.91E-001	1.1E-002	7.91
Total removal	9.21E+000	1.2E-001	92.09
Total biodegradation	9.16E+000	1.2E-001	91.65

## Level III Fugacity Model (Full-Output):

```

=====
Chem Name      :
Molecular Wt: 74.12
Henry's LC   : 9.99e-006 atm-m3/mole (Henrywin program)
Vapor Press  : 89.6 mm Hg (Mpppwin program)
Log Kow      : 0.73 (Kowwin program)
Soil Koc     : 2.2 (calc by model)

```

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	7.17	152	1000
Water	43.5	360	1000
Soil	49.3	720	1000
Sediment	0.0836	3.24e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	2.54e-010	352	771	11.7	25.7
Water	3.15e-010	900	468	30	15.6
Soil	1.12e-008	510	0	17	0
Sediment	2.88e-010	0.192	0.018	0.00641	0.000599

```

Persistence Time: 358 hr
Reaction Time:    610 hr
Advection Time:   868 hr
Percent Reacted:  58.7
Percent Advected: 41.3

```

## Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

```

Air:    151.8
Water:  360
Soil:   720
Sediment: 3240
Biowin estimate: 2.823 (weeks )

```

## Advection Times (hr):

```

Air:    100
Water:  1000
Sediment: 5e+004

```

## APPENDIX II

### EUSES (V2.03) REPORT

### TERT-BUTYL ALCOHOL

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The following default values were replaced in the EUSES calculation:

- For all scenarios the use of an STP was assumed for the marine compartment.
- Release fractions were set on the basis of tert-butyl alcohol distribution modelling:

Scenario	Release fraction Air	Release Fraction Water	Release Fraction Sediment
Use 0: Production	0.0959	0.9038	0.0002
Use 1: Reagent in chemical synthesis	0.0959	0.9038	0.0002

- The number of emission days was set to 292 days for all scenarios, based on the assumption of an average utilisation of 80%. This figure is considered to represent a worst case situation.
-

**PHYSICO-CHEMICAL PROPERTIES**

MELTING POINT	25.3	[OC]	S	
BOILING POINT	82.8	[OC]	S	
VAPOUR PRESSURE AT TEST TEMPERATURE	40.7	[HPA]	S	
TEMPERATURE AT WHICH VAPOUR PRESSURE WAS MEASURED		20	[OC]	S
VAPOUR PRESSURE AT 25 [OC]	5.74E+03	[PA]	O	
WATER SOLUBILITY AT TEST TEMPERATURE	1E+05	[MG.L-1]	S	
TEMPERATURE AT WHICH SOLUBILITY WAS MEASURED	25	[OC]	S	
WATER SOLUBILITY AT 25 [OC]	1E+05	[MG.L-1]	O	
OCTANOL-WATER PARTITION COEFFICIENT	0.3	[LOG10]	S	
HENRY'S LAW CONSTANT	4.26	[PA.M3.MOL-1]	O	

**ENVIRONMENT-EXPOSURE****RELEASE ESTIMATION**

TONNAGE OF SUBSTANCE IN EUROPE	50	[TONNES.YR-1]	O
REGIONAL PRODUCTION VOLUME OF SUBSTANCE	50	[TONNES.YR-1]	O

**ENVIRONMENT-EXPOSURE****RELEASE ESTIMATION****[1 "USE 0: PRODUCTION", IC=15/UC=55]**

INDUSTRY CATEGORY	15/0 OTHERS		S
USE CATEGORY	55/0 OTHERS		S
FRACTION OF TONNAGE FOR APPLICATION	1	[-]	O

**ENVIRONMENT-EXPOSURE****RELEASE ESTIMATION****[PRODUCTION]**

USE SPECIFIC EMISSION SCENARIO	NO		D
EMISSION TABLES	A1.1 (GENERAL TABLE), B1.2 (SPECIFIC USES)		S
EMISSION SCENARIO	NO SPECIAL SCENARIO SELECTED/AVAILABLE		S
MAIN CATEGORY PRODUCTION	IC INTERMED. STORED OFF-SITE/DEDICATED EQUIP.		S
FRACTION OF TONNAGE RELEASED TO AIR	0.09588	[-]	S
FRACTION OF TONNAGE RELEASED TO WASTE WATER	0.90382	[-]	S
FRACTION OF TONNAGE RELEASED TO SURFACEWATER	0	[-]	S
FRACTION OF TONNAGE RELEASED TO INDUSTRIAL SOIL	1.6E-04	[-]	S
FRACTION OF TONNAGE RELEASED TO AGRICULTURAL SOIL	0	[-]	S
FRACTION OF THE MAIN LOCAL SOURCE	1	[-]	S
NUMBER OF EMISSION DAYS PER YEAR	292	[-]	S
LOCAL EMISSION TO AIR DURING EPISODE	16.4	[KG.D-1]	O
LOCAL EMISSION TO WASTEWATER DURING EPISODE	155	[KG.D-1]	O
INTERMITTENT RELEASE	NO		D

**ENVIRONMENT-EXPOSURE****RELEASE ESTIMATION****[2 "USE 1: REAGENT IN CHEMICAL SYNTHESIS", IC=3/UC=55]**

INDUSTRY CATEGORY	3 CHEMICAL INDUSTRY: CHEMICALS USED IN SYNTHESIS		S
USE CATEGORY	55/0 OTHERS		S
FRACTION OF TONNAGE FOR APPLICATION	1	[-]	O

**ENVIRONMENT-EXPOSURE****RELEASE ESTIMATION****[INDUSTRIAL USE]**

USE SPECIFIC EMISSION SCENARIO	NO		D
EMISSION TABLES	A3.3 (IC-SPECIFIC), B3.2 (GENERAL TABLE)		S
EMISSION SCENARIO	NO SPECIAL SCENARIO SELECTED/AVAILABLE		S
MAIN CATEGORY INDUSTRIAL USE	III NON-DISPERSIVE USE		S
FRACTION OF TONNAGE RELEASED TO AIR	0.025	[-]	O
FRACTION OF TONNAGE RELEASED TO WASTE WATER	0.02	[-]	O
FRACTION OF TONNAGE RELEASED TO SURFACEWATER	0	[-]	O
FRACTION OF TONNAGE RELEASED TO INDUSTRIAL SOIL	1E-04	[-]	O
FRACTION OF TONNAGE RELEASED TO AGRICULTURAL SOIL	0	[-]	O
FRACTION OF THE MAIN LOCAL SOURCE	0.5	[-]	O
NUMBER OF EMISSION DAYS PER YEAR	10	[-]	O
LOCAL EMISSION TO AIR DURING EPISODE	62.5	[KG.D-1]	O
LOCAL EMISSION TO WASTEWATER DURING EPISODE	50	[KG.D-1]	O
INTERMITTENT RELEASE	NO		D

**ENVIRONMENT-EXPOSURE****RELEASE ESTIMATION****TOTAL REGIONAL EMISSIONS TO COMPARTMENTS**

TOTAL REGIONAL EMISSION TO AIR	16.6	[KG.D-1]	O
TOTAL REGIONAL EMISSION TO WASTEWATER	101	[KG.D-1]	O
TOTAL REGIONAL EMISSION TO SURFACE WATER	25.3	[KG.D-1]	O
TOTAL REGIONAL EMISSION TO INDUSTRIAL SOIL	0.0356	[KG.D-1]	O
TOTAL REGIONAL EMISSION TO AGRICULTURAL SOIL	0	[KG.D-1]	O

**ENVIRONMENT-EXPOSURE****DEGRADATION AND TRANSFORMATION**

CHARACTERIZATION OF BIODEGRADABILITY	NOT BIODEGRADABLE		D
DEGRADATION CALCULATION METHOD IN STP	FIRST ORDER, STANDARD OECD/EU TESTS		D
RATE CONSTANT FOR BIODEGRADATION IN STP	0	[D-1]	O
RATE CONSTANT FOR BIODEGRADATION IN SURFACE WATER	0	[D-1] (12[OC])	O
RATE CONSTANT FOR BIODEGRADATION IN BULK SOIL	6.93E-07	[D-1] (12[OC])	O
RATE CONSTANT FOR BIODEGRADATION IN AERATED SEDIMENT	6.93E-07	[D-1] (12[OC])	O
RATE CONSTANT FOR HYDROLYSIS IN SURFACE WATER	6.93E-07	[D-1] (12[OC])	O
RATE CONSTANT FOR PHOTOLYSIS IN SURFACE WATER	6.93E-07	[D-1]	O

## ENVIRONMENT-EXPOSURE

## SEWAGE TREATMENT

## LOCAL STP [1 "USE 0: PRODUCTION", IC=15/UC=55][PRODUCTION]

## OUTPUT

FRACTION OF EMISSION DIRECTED TO AIR BY STP	7.39	[%]	O	
FRACTION OF EMISSION DIRECTED TO WATER BY STP	92.4	[%]	O	
FRACTION OF EMISSION DIRECTED TO SLUDGE BY STP	0.184	[%]	O	
FRACTION OF THE EMISSION DEGRADED IN STP	0	[%]	O	
CONCENTRATION IN UNTREATED WASTEWATER	77.4	[MG.L-1]	O	
CONCENTRATION OF CHEMICAL (TOTAL) IN THE STP-EFFLUENT	71.5	[MG.L-1]	O	O
CONCENTRATION IN EFFLUENT EXCEEDS SOLUBILITY	NO		O	
CONCENTRATION IN DRY SEWAGE SLUDGE	361	[MG.KG-1]	O	
PEC FOR MICRO-ORGANISMS IN THE STP	71.5	[MG.L-1]	O	

## ENVIRONMENT-EXPOSURE

## SEWAGE TREATMENT

## LOCAL STP [2 "USE 1: REAGENT IN CHEMICAL SYNTHESIS", IC=3/UC=55][INDUSTRIAL USE]

## OUTPUT

FRACTION OF EMISSION DIRECTED TO AIR BY STP	7.39	[%]	O	
FRACTION OF EMISSION DIRECTED TO WATER BY STP	92.4	[%]	O	
FRACTION OF EMISSION DIRECTED TO SLUDGE BY STP	0.184	[%]	O	
FRACTION OF THE EMISSION DEGRADED IN STP	0	[%]	O	
CONCENTRATION IN UNTREATED WASTEWATER	25	[MG.L-1]	O	
CONCENTRATION OF CHEMICAL (TOTAL) IN THE STP-EFFLUENT	23.1	[MG.L-1]	O	O
CONCENTRATION IN EFFLUENT EXCEEDS SOLUBILITY	NO		O	
CONCENTRATION IN DRY SEWAGE SLUDGE	117	[MG.KG-1]	O	
PEC FOR MICRO-ORGANISMS IN THE STP	23.1	[MG.L-1]	O	

## ENVIRONMENT-EXPOSURE

## DISTRIBUTION

## LOCAL SCALE

## [1 "USE 0: PRODUCTION", IC=15/UC=55][PRODUCTION]

CONCENTRATION IN AIR DURING EMISSION EPISODE	4.56E-03	[MG.M-3]	O	
ANNUAL AVERAGE CONCENTRATION IN AIR, 100 M FROM POINT SOURCE	3.65E-03	[MG.M-3]	O	
CONCENTRATION IN SURFACE WATER DURING EMISSION EPISODE (DISSOLVED)	7.15	[MG.L-1]	O	O
ANNUAL AVERAGE CONCENTRATION IN SURFACE WATER (DISSOLVED)	5.72	[MG.L-1]	O	
LOCAL PEC IN SURFACE WATER DURING EMISSION EPISODE (DISSOLVED)	7.15	[MG.L-1]	O	
ANNUAL AVERAGE LOCAL PEC IN SURFACE WATER (DISSOLVED)	5.72	[MG.L-1]	O	
LOCAL PEC IN FRESH-WATER SEDIMENT DURING EMISSION EPISODE	7.93	[MG.KGWWT-1]	O	
CONCENTRATION IN SEA WATER DURING EMISSION EPISODE (DISSOLVED)	0.774	[MG.L-1]	O	
ANNUAL AVERAGE CONCENTRATION IN SEA WATER (DISSOLVED)	0.619	[MG.L-1]	O	
LOCAL PEC IN SEA WATER DURING EMISSION EPISODE (DISSOLVED)	0.774	[MG.L-1]	O	
ANNUAL AVERAGE LOCAL PEC IN SEA WATER (DISSOLVED)	0.619	[MG.L-1]	O	
LOCAL PEC IN MARINE SEDIMENT DURING EMISSION EPISODE	0.858	[MG.KGWWT-1]	O	
LOCAL PEC IN AGRIC. SOIL (TOTAL) AVERAGED OVER 30 DAYS	0.467	[MG.KGWWT-1]	O	
LOCAL PEC IN AGRIC. SOIL (TOTAL) AVERAGED OVER 180 DAYS	0.244	[MG.KGWWT-1]	O	
LOCAL PEC IN GRASSLAND (TOTAL) AVERAGED OVER 180 DAYS	0.0567	[MG.KGWWT-1]	O	
LOCAL PEC IN GROUNDWATER UNDER AGRICULTURAL SOIL	0.637	[MG.L-1]	O	

## ENVIRONMENT-EXPOSURE

## DISTRIBUTION

## LOCAL SCALE

## [2 "USE 1: REAGENT IN CHEMICAL SYNTHESIS", IC=3/UC=55][INDUSTRIAL USE]

CONCENTRATION IN AIR DURING EMISSION EPISODE	0.0174	[MG.M-3]	O	
ANNUAL AVERAGE CONCENTRATION IN AIR, 100 M FROM POINT SOURCE	4.76E-04	[MG.M-3]	O	
CONCENTRATION IN SURFACE WATER DURING EMISSION EPISODE (DISSOLVED)	2.31	[MG.L-1]	O	O
ANNUAL AVERAGE CONCENTRATION IN SURFACE WATER (DISSOLVED)	0.0633	[MG.L-1]	O	
LOCAL PEC IN SURFACE WATER DURING EMISSION EPISODE (DISSOLVED)	2.31	[MG.L-1]	O	
ANNUAL AVERAGE LOCAL PEC IN SURFACE WATER (DISSOLVED)	0.0636	[MG.L-1]	O	
LOCAL PEC IN FRESH-WATER SEDIMENT DURING EMISSION EPISODE	2.56	[MG.KGWWT-1]	O	
CONCENTRATION IN SEA WATER DURING EMISSION EPISODE (DISSOLVED)	0.25	[MG.L-1]	O	
ANNUAL AVERAGE CONCENTRATION IN SEA WATER (DISSOLVED)	6.85E-03	[MG.L-1]	O	
LOCAL PEC IN SEA WATER DURING EMISSION EPISODE (DISSOLVED)	0.25	[MG.L-1]	O	
ANNUAL AVERAGE LOCAL PEC IN SEA WATER (DISSOLVED)	6.88E-03	[MG.L-1]	O	
LOCAL PEC IN MARINE SEDIMENT DURING EMISSION EPISODE	0.277	[MG.KGWWT-1]	O	
LOCAL PEC IN AGRIC. SOIL (TOTAL) AVERAGED OVER 30 DAYS	0.15	[MG.KGWWT-1]	O	
LOCAL PEC IN AGRIC. SOIL (TOTAL) AVERAGED OVER 180 DAYS	0.0782	[MG.KGWWT-1]	O	
LOCAL PEC IN GRASSLAND (TOTAL) AVERAGED OVER 180 DAYS	0.0177	[MG.KGWWT-1]	O	
LOCAL PEC IN GROUNDWATER UNDER AGRICULTURAL SOIL	0.204	[MG.L-1]	O	



**ENVIRONMENT-EXPOSURE****DISTRIBUTION****REGIONAL AND CONTINENTAL SCALE****CONTINENTAL**

CONTINENTAL PEC IN SURFACE WATER (DISSOLVED)	5.35E-07	[MG.L-1]	O	
CONTINENTAL PEC IN SEA WATER (DISSOLVED)	4.91E-07	[MG.L-1]	O	
CONTINENTAL PEC IN AIR (TOTAL)	4.42E-07	[MG.M-3]	O	
CONTINENTAL PEC IN AGRICULTURAL SOIL (TOTAL)	3.28E-07	[MG.KGWWT-1]	O	
CONTINENTAL PEC IN PORE WATER OF AGRICULTURAL SOILS	8.57E-07	[MG.L-1]	O	O
CONTINENTAL PEC IN NATURAL SOIL (TOTAL)	3.28E-07	[MG.KGWWT-1]	O	
CONTINENTAL PEC IN INDUSTRIAL SOIL (TOTAL)	3.28E-07	[MG.KGWWT-1]	O	
CONTINENTAL PEC IN SEDIMENT (TOTAL)	5.4E-07	[MG.KGWWT-1]	O	
CONTINENTAL PEC IN SEA WATER SEDIMENT (TOTAL)	5E-07	[MG.KGWWT-1]	O	

**ENVIRONMENT-EXPOSURE****DISTRIBUTION****REGIONAL AND CONTINENTAL SCALE****REGIONAL**

REGIONAL PEC IN SURFACE WATER (DISSOLVED)	3.3E-04	[MG.L-1]	O	
REGIONAL PEC IN SEA WATER (DISSOLVED)	2.97E-05	[MG.L-1]	O	
REGIONAL PEC IN AIR (TOTAL)	2.45E-06	[MG.M-3]	O	
REGIONAL PEC IN AGRICULTURAL SOIL (TOTAL)	3.89E-06	[MG.KGWWT-1]	O	
REGIONAL PEC IN PORE WATER OF AGRICULTURAL SOILS	1.02E-05	[MG.L-1]	O	
REGIONAL PEC IN NATURAL SOIL (TOTAL)	1.81E-06	[MG.KGWWT-1]	O	
REGIONAL PEC IN INDUSTRIAL SOIL (TOTAL)	4.18E-06	[MG.KGWWT-1]	O	
REGIONAL PEC IN SEDIMENT (TOTAL)	3.33E-04	[MG.KGWWT-1]	O	
REGIONAL PEC IN SEA WATER SEDIMENT (TOTAL)	3.02E-05	[MG.KGWWT-1]	O	

**ENVIRONMENT-EXPOSURE****BIOCONCENTRATION**

BIOCONCENTRATION FACTOR FOR EARTHWORMS	0.864	[L.KGWWT-1]	O	
BIOCONCENTRATION FACTOR FOR FISH	1.41	[L.KGWWT-1]	O	

**ENVIRONMENT-EXPOSURE****SECONDARY POISONING [1 "USE 0: PRODUCTION", IC=15/UC=55][PRODUCTION]**

CONCENTRATION IN FISH FOR SECONDARY POISONING (FRESH WATER)	4.04	[MG.KGWWT-1]	O	
CONCENTRATION IN FISH FOR SECONDARY POISONING (MARINE)	0.437	[MG.KGWWT-1]	O	
CONCENTRATION IN FISH-EATING MARINE TOP-PREDATORS	0.0875	[MG.KGWWT-1]	O	
CONCENTRATION IN EARTHWORMS FROM AGRICULTURAL SOIL	0.26	[MG.KG-1]	O	

**ENVIRONMENT-EXPOSURE****SECONDARY POISONING [2 "USE 1: REAGENT IN CHEMICAL SYNTHESIS", IC=3/UC=55][INDUSTRIAL USE]**

CONCENTRATION IN FISH FOR SECONDARY POISONING (FRESH WATER)	0.0452	[MG.KGWWT-1]	O	
CONCENTRATION IN FISH FOR SECONDARY POISONING (MARINE)	4.88E-03	[MG.KGWWT-1]	O	
CONCENTRATION IN FISH-EATING MARINE TOP-PREDATORS	1.01E-03	[MG.KGWWT-1]	O	
CONCENTRATION IN EARTHWORMS FROM AGRICULTURAL SOIL	0.0833	[MG.KG-1]	O	



**ENVIRONMENT - EFFECTS****MICRO-ORGANISMS**

TEST SYSTEM	RESPIRATION INHIBITION, EU ANNEX V C.11, OECD 209		D	
EC50 FOR MICRO-ORGANISMS IN A STP	??	[MG.L-1]	D	
EC10 FOR MICRO-ORGANISMS IN A STP	??	[MG.L-1]	D	
NOEC FOR MICRO-ORGANISMS IN A STP	??	[MG.L-1]	D	
PNEC FOR MICRO-ORGANISMS IN A STP	??	[MG.L-1]	O	
ASSESSMENT FACTOR APPLIED IN EXTRAPOLATION TO PNEC MICRO	??		[-]	O

**ENVIRONMENT - EFFECTS****FRESH WATER ORGANISMS**

LC50 FOR FISH	??	[MG.L-1]	D	
L(E)C50 FOR DAPHNIA	??	[MG.L-1]	D	
EC50 FOR ALGAE	??	[MG.L-1]	D	
LC50 FOR ADDITIONAL TAXONOMIC GROUP	??	[MG.L-1]	D	
NOEC FOR FISH	??	[MG.L-1]	D	
NOEC FOR DAPHNIA	??	[MG.L-1]	D	
NOEC FOR ALGAE	??	[MG.L-1]	D	
NOEC FOR ADDITIONAL TAXONOMIC GROUP	??	[MG.L-1]	D	
PNEC FOR AQUATIC ORGANISMS	??	[MG.L-1]	O	
PNEC FOR AQUATIC ORGANISMS, INTERMITTENT RELEASES??		[MG.L-1]	O	

**ENVIRONMENT - EFFECTS****MARINE ORGANISMS**

LC50 FOR FISH (MARINE)	??	[MG.L-1]	D	
L(E)C50 FOR CRUSTACEANS (MARINE)	??	[MG.L-1]	D	
EC50 FOR ALGAE (MARINE)	??	[MG.L-1]	D	
LC50 FOR ADDITIONAL TAXONOMIC GROUP (MARINE)	??	[MG.L-1]	D	
NOEC FOR FISH (MARINE)	??	[MG.L-1]	D	
NOEC FOR CRUSTACEANS (MARINE)	??	[MG.L-1]	D	
NOEC FOR ALGAE (MARINE)	??	[MG.L-1]	D	
NOEC FOR ADDITIONAL TAXONOMIC GROUP (MARINE)	??	[MG.L-1]	D	
PNEC FOR MARINE ORGANISMS	??	[MG.L-1]	O	

**ENVIRONMENT - EFFECTS****FRESH-WATER SEDIMENT ORGANISMS**

LC50 FOR FRESH-WATER SEDIMENT ORGANISM	??	[MG.KGWWT-1]	D	
EC10 FOR FRESH-WATER SEDIMENT ORGANISM	??	[MG.KGWWT-1]	D	
EC10 FOR FRESH-WATER SEDIMENT ORGANISM	??	[MG.KGWWT-1]	D	
EC10 FOR FRESH-WATER SEDIMENT ORGANISM	??	[MG.KGWWT-1]	D	
NOEC FOR FRESH-WATER SEDIMENT ORGANISM	??	[MG.KGWWT-1]	D	
NOEC FOR FRESH-WATER SEDIMENT ORGANISM	??	[MG.KGWWT-1]	D	
NOEC FOR FRESH-WATER SEDIMENT ORGANISM	??	[MG.KGWWT-1]	D	
PNEC FOR FRESH-WATER SEDIMENT-DWELLING ORGANISMS	??		[MG.KGWWT-1]	O

**ENVIRONMENT - EFFECTS****MARINE SEDIMENT ORGANISMS**

LC50 FOR MARINE SEDIMENT ORGANISM	??	[MG.KGWWT-1]	D	
EC10 FOR MARINE SEDIMENT ORGANISM	??	[MG.KGWWT-1]	D	
EC10 FOR MARINE SEDIMENT ORGANISM	??	[MG.KGWWT-1]	D	
EC10 FOR MARINE SEDIMENT ORGANISM	??	[MG.KGWWT-1]	D	
NOEC FOR MARINE SEDIMENT ORGANISM	??	[MG.KGWWT-1]	D	
NOEC FOR MARINE SEDIMENT ORGANISM	??	[MG.KGWWT-1]	D	
NOEC FOR MARINE SEDIMENT ORGANISM	??	[MG.KGWWT-1]	D	
PNEC FOR MARINE SEDIMENT ORGANISMS	??	[MG.KGWWT-1]	O	

**ENVIRONMENT - EFFECTS****TERRESTRIAL ORGANISMS**

LC50 FOR PLANTS	??	[MG.KGWWT-1]	D	
LC50 FOR EARTHWORMS	??	[MG.KGWWT-1]	D	
EC50 FOR MICROORGANISMS	??	[MG.KGWWT-1]	D	
LC50 FOR OTHER TERRESTRIAL SPECIES	??	[MG.KGWWT-1]	D	
NOEC FOR PLANTS	??	[MG.KGWWT-1]	D	
NOEC FOR EARTHWORMS	??	[MG.KGWWT-1]	D	
NOEC FOR MICROORGANISMS	??	[MG.KGWWT-1]	D	
NOEC FOR ADDITIONAL TAXONOMIC GROUP	??	[MG.KGWWT-1]	D	
NOEC FOR ADDITIONAL TAXONOMIC GROUP	??	[MG.KGWWT-1]	D	
PNEC FOR TERRESTRIAL ORGANISMS	??	[MG.KGWWT-1]	O	
EQUILIBRIUM PARTITIONING USED FOR PNEC IN SOIL?	YES		O	

**ENVIRONMENT - EFFECTS****BIRDS AND MAMMALS**

DURATION OF (SUB-)CHRONIC ORAL TEST	28 DAYS		D	
NOEC VIA FOOD FOR SECONDARY POISONING	??	[MG.KG-1]	O	
PNEC FOR SECONDARY POISONING OF BIRDS AND MAMMALS	??		[MG.KG-1]	O

**ENVIRONMENT - RISK CHARACTERIZATION****LOCAL [1 "USE 0: PRODUCTION", IC=15/UC=55][PRODUCTION]**

RCR FOR THE LOCAL FRESH-WATER COMPARTMENT	??	[-]	O	
RCR FOR THE LOCAL FRESH-WATER COMPARTMENT, STATISTICAL METHOD	??	[-]		O
RCR FOR THE LOCAL MARINE COMPARTMENT	??	[-]	O	
RCR FOR THE LOCAL MARINE COMPARTMENT, STATISTICAL METHOD	??	[-]		O
RCR FOR THE LOCAL FRESH-WATER SEDIMENT COMPARTMENT	??	[-]		O
RCR FOR THE LOCAL MARINE SEDIMENT COMPARTMENT	??	[-]	O	
RCR FOR THE LOCAL SOIL COMPARTMENT	??	[-]	O	
RCR FOR THE LOCAL SOIL COMPARTMENT, STATISTICAL METHOD	??	[-]		O
RCR FOR THE SEWAGE TREATMENT PLANT	??	[-]	O	
RCR FOR FISH-EATING BIRDS AND MAMMALS (FRESH-WATER)	??	[-]		O
RCR FOR FISH-EATING BIRDS AND MAMMALS (MARINE)	??	[-]	O	
RCR FOR TOP PREDATORS (MARINE)	??	[-]	O	
RCR FOR WORM-EATING BIRDS AND MAMMALS	??	[-]	O	

**ENVIRONMENT - RISK CHARACTERIZATION****LOCAL [2 "USE 1: REAGENT IN CHEMICAL SYNTHESIS", IC=3/UC=55][INDUSTRIAL USE]**

RCR FOR THE LOCAL FRESH-WATER COMPARTMENT	??	[-]	O	
RCR FOR THE LOCAL FRESH-WATER COMPARTMENT, STATISTICAL METHOD	??	[-]		O
RCR FOR THE LOCAL MARINE COMPARTMENT	??	[-]	O	
RCR FOR THE LOCAL MARINE COMPARTMENT, STATISTICAL METHOD	??	[-]		O
RCR FOR THE LOCAL FRESH-WATER SEDIMENT COMPARTMENT	??	[-]		O
RCR FOR THE LOCAL MARINE SEDIMENT COMPARTMENT	??	[-]	O	
RCR FOR THE LOCAL SOIL COMPARTMENT	??	[-]	O	
RCR FOR THE LOCAL SOIL COMPARTMENT, STATISTICAL METHOD	??	[-]		O
RCR FOR THE SEWAGE TREATMENT PLANT	??	[-]	O	
RCR FOR FISH-EATING BIRDS AND MAMMALS (FRESH-WATER)	??	[-]		O
RCR FOR FISH-EATING BIRDS AND MAMMALS (MARINE)	??	[-]	O	
RCR FOR TOP PREDATORS (MARINE)	??	[-]	O	
RCR FOR WORM-EATING BIRDS AND MAMMALS	??	[-]	O	

**ENVIRONMENT - RISK CHARACTERIZATION****REGIONAL**

RCR FOR THE REGIONAL FRESH-WATER COMPARTMENT	??	[-]	O	
RCR FOR THE REGIONAL FRESH-WATER COMPARTMENT, STATISTICAL METHOD	??	[-]		O
RCR FOR THE REGIONAL MARINE COMPARTMENT	??	[-]	O	
RCR FOR THE REGIONAL MARINE COMPARTMENT, STATISTICAL METHOD	??	[-]		O
RCR FOR THE REGIONAL FRESH-WATER SEDIMENT COMPARTMENT	??	[-]		O
RCR FOR THE REGIONAL MARINE SEDIMENT COMPARTMENT	??	[-]	O	
RCR FOR THE REGIONAL SOIL COMPARTMENT	??	[-]	O	
RCR FOR THE REGIONAL SOIL COMPARTMENT, STATISTICAL METHOD	??	[-]		O

**HUMAN HEALTH - EXPOSURE ASSESSMENT****HUMANS EXPOSED VIA THE ENVIRONMENT****LOCAL SCALE**

PURIFICATION FACTOR FOR SURFACE WATER	1	[-]	O
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**HUMAN HEALTH - EXPOSURE ASSESSMENT****HUMANS EXPOSED VIA THE ENVIRONMENT****LOCAL SCALE****CONCENTRATIONS IN INTAKE MEDIA [1 "USE 0: PRODUCTION", IC=15/UC=55][PRODUCTION]**

LOCAL CONCENTRATION IN WET FISH	8.08	[MG.KG-1]	O
LOCAL CONCENTRATION IN ROOT TISSUE OF PLANT	0.61	[MG.KG-1]	O
LOCAL CONCENTRATION IN LEAVES OF PLANT	2.2E-03	[MG.KG-1]	O
LOCAL CONCENTRATION IN GRASS (WET WEIGHT)	2E-03	[MG.KG-1]	O
LOCAL CONCENTRATION IN DRINKING WATER	5.72	[MG.L-1]	O
LOCAL CONCENTRATION IN MEAT (WET WEIGHT)	2.5E-04	[MG.KG-1]	O
LOCAL CONCENTRATION IN MILK (WET WEIGHT)	2.5E-03	[MG.KG-1]	O

**HUMAN HEALTH - EXPOSURE ASSESSMENT****HUMANS EXPOSED VIA THE ENVIRONMENT****LOCAL SCALE****DOSES IN INTAKE MEDIA [1 "USE 0: PRODUCTION", IC=15/UC=55][PRODUCTION]**

DAILY DOSE THROUGH INTAKE OF DRINKING WATER	0.163	[MG.KG-1.D-1]	O
DAILY DOSE THROUGH INTAKE OF FISH	0.0133	[MG.KG-1.D-1]	O
DAILY DOSE THROUGH INTAKE OF LEAF CROPS	3.77E-05	[MG.KG-1.D-1]	O
DAILY DOSE THROUGH INTAKE OF ROOT CROPS	3.34E-03	[MG.KG-1.D-1]	O
DAILY DOSE THROUGH INTAKE OF MEAT	1.08E-06	[MG.KG-1.D-1]	O
DAILY DOSE THROUGH INTAKE OF MILK	2.01E-05	[MG.KG-1.D-1]	O
DAILY DOSE THROUGH INTAKE OF AIR	1.04E-03	[MG.KG-1.D-1]	O

**HUMAN HEALTH - EXPOSURE ASSESSMENT****HUMANS EXPOSED VIA THE ENVIRONMENT****LOCAL SCALE****FRACTIONS OF TOTAL DOSE [1 "USE 0: PRODUCTION", IC=15/UC=55][PRODUCTION]**

FRACTION OF TOTAL DOSE THROUGH INTAKE OF DRINKING WATER	0.902	[-]	O
FRACTION OF TOTAL DOSE THROUGH INTAKE OF FISH	0.0733	[-]	O
FRACTION OF TOTAL DOSE THROUGH INTAKE OF LEAF CROPS	2.08E-04	[-]	O
FRACTION OF TOTAL DOSE THROUGH INTAKE OF ROOT CROPS	0.0185	[-]	O
FRACTION OF TOTAL DOSE THROUGH INTAKE OF MEAT	5.94E-06	[-]	O
FRACTION OF TOTAL DOSE THROUGH INTAKE OF MILK	1.11E-04	[-]	O
FRACTION OF TOTAL DOSE THROUGH INTAKE OF AIR	5.76E-03	[-]	O
LOCAL TOTAL DAILY INTAKE FOR HUMANS	0.181	[MG.KG-1.D-1]	O

**HUMAN HEALTH - EXPOSURE ASSESSMENT****HUMANS EXPOSED VIA THE ENVIRONMENT****LOCAL SCALE****CONCENTRATIONS IN INTAKE MEDIA [2 "USE 1: REAGENT IN CHEMICAL SYNTHESIS", IC=3/UC=55][INDUSTRIAL USE]**

LOCAL CONCENTRATION IN WET FISH	0.0899	[MG.KG-1]	O
LOCAL CONCENTRATION IN ROOT TISSUE OF PLANT	0.195	[MG.KG-1]	O
LOCAL CONCENTRATION IN LEAVES OF PLANT	3.35E-04	[MG.KG-1]	O
LOCAL CONCENTRATION IN GRASS (WET WEIGHT)	2.73E-04	[MG.KG-1]	O
LOCAL CONCENTRATION IN DRINKING WATER	0.204	[MG.L-1]	O
LOCAL CONCENTRATION IN MEAT (WET WEIGHT)	9E-06	[MG.KG-1]	O
LOCAL CONCENTRATION IN MILK (WET WEIGHT)	9E-05	[MG.KG-1]	O

**HUMAN HEALTH - EXPOSURE ASSESSMENT****HUMANS EXPOSED VIA THE ENVIRONMENT****LOCAL SCALE****DOSES IN INTAKE MEDIA [2 "USE 1: REAGENT IN CHEMICAL SYNTHESIS", IC=3/UC=55][INDUSTRIAL USE]**

DAILY DOSE THROUGH INTAKE OF DRINKING WATER	5.84E-03	[MG.KG-1.D-1]	O
DAILY DOSE THROUGH INTAKE OF FISH	1.48E-04	[MG.KG-1.D-1]	O
DAILY DOSE THROUGH INTAKE OF LEAF CROPS	5.75E-06	[MG.KG-1.D-1]	O
DAILY DOSE THROUGH INTAKE OF ROOT CROPS	1.07E-03	[MG.KG-1.D-1]	O
DAILY DOSE THROUGH INTAKE OF MEAT	3.87E-08	[MG.KG-1.D-1]	O
DAILY DOSE THROUGH INTAKE OF MILK	7.21E-07	[MG.KG-1.D-1]	O
DAILY DOSE THROUGH INTAKE OF AIR	1.37E-04	[MG.KG-1.D-1]	O

**HUMAN HEALTH - EXPOSURE ASSESSMENT****HUMANS EXPOSED VIA THE ENVIRONMENT****LOCAL SCALE****FRACTIONS OF TOTAL DOSE [2 "USE 1: REAGENT IN CHEMICAL SYNTHESIS", IC=3/UC=55][INDUSTRIAL USE]**

FRACTION OF TOTAL DOSE THROUGH INTAKE OF DRINKING WATER	0.811	[-]	O
FRACTION OF TOTAL DOSE THROUGH INTAKE OF FISH	0.0205	[-]	O
FRACTION OF TOTAL DOSE THROUGH INTAKE OF LEAF CROPS	7.98E-04	[-]	O
FRACTION OF TOTAL DOSE THROUGH INTAKE OF ROOT CROPS	0.149	[-]	O
FRACTION OF TOTAL DOSE THROUGH INTAKE OF MEAT	5.37E-06	[-]	O
FRACTION OF TOTAL DOSE THROUGH INTAKE OF MILK	1E-04	[-]	O
FRACTION OF TOTAL DOSE THROUGH INTAKE OF AIR	0.019	[-]	O
LOCAL TOTAL DAILY INTAKE FOR HUMANS	7.2E-03	[MG.KG-1.D-1]	O

**HUMAN HEALTH - EXPOSURE ASSESSMENT****HUMANS EXPOSED VIA THE ENVIRONMENT****REGIONAL SCALE****CONCENTRATIONS IN INTAKE MEDIA**

REGIONAL CONCENTRATION IN WET FISH	4.67E-04	[MG.KG-1]	O
REGIONAL CONCENTRATION IN ROOT TISSUE OF PLANT	9.72E-06	[MG.KG-1]	O
REGIONAL CONCENTRATION IN LEAVES OF PLANT	1.31E-06	[MG.KG-1]	O
REGIONAL CONCENTRATION IN GRASS (WET WEIGHT)	1.31E-06	[MG.KG-1]	O
REGIONAL CONCENTRATION IN DRINKING WATER	3.3E-04	[MG.L-1]	O
REGIONAL CONCENTRATION IN MEAT (WET WEIGHT)	1.47E-08	[MG.KG-1]	O
REGIONAL CONCENTRATION IN MILK (WET WEIGHT)	1.47E-07	[MG.KG-1]	O

**HUMAN HEALTH - EXPOSURE ASSESSMENT****HUMANS EXPOSED VIA THE ENVIRONMENT****REGIONAL SCALE****DOSES IN INTAKE MEDIA**

DAILY DOSE THROUGH INTAKE OF DRINKING WATER	9.44E-06	[MG.KG-1.D-1]	O
DAILY DOSE THROUGH INTAKE OF FISH	7.67E-07	[MG.KG-1.D-1]	O
DAILY DOSE THROUGH INTAKE OF LEAF CROPS	2.24E-08	[MG.KG-1.D-1]	O
DAILY DOSE THROUGH INTAKE OF ROOT CROPS	5.33E-08	[MG.KG-1.D-1]	O
DAILY DOSE THROUGH INTAKE OF MEAT	6.34E-11	[MG.KG-1.D-1]	O
DAILY DOSE THROUGH INTAKE OF MILK	1.18E-09	[MG.KG-1.D-1]	O
DAILY DOSE THROUGH INTAKE OF AIR	6.99E-07	[MG.KG-1.D-1]	O

**HUMAN HEALTH - EXPOSURE ASSESSMENT****HUMANS EXPOSED VIA THE ENVIRONMENT****REGIONAL SCALE****FRACTIONS OF TOTAL DOSE**

FRACTION OF TOTAL DOSE THROUGH INTAKE OF DRINKING WATER	0.86	[-]	O
FRACTION OF TOTAL DOSE THROUGH INTAKE OF FISH	0.0698	[-]	O
FRACTION OF TOTAL DOSE THROUGH INTAKE OF LEAF CROPS	2.04E-03	[-]	O
FRACTION OF TOTAL DOSE THROUGH INTAKE OF ROOT CROPS	4.86E-03	[-]	O
FRACTION OF TOTAL DOSE THROUGH INTAKE OF MEAT	5.77E-06	[-]	O
FRACTION OF TOTAL DOSE THROUGH INTAKE OF MILK	1.08E-04	[-]	O
FRACTION OF TOTAL DOSE THROUGH INTAKE OF AIR	0.0636	[-]	O
REGIONAL TOTAL DAILY INTAKE FOR HUMANS	1.1E-05	[MG.KG-1.D-1]	O

**HUMAN HEALTH - RISK CHARACTERIZATION****CURRENT CLASSIFICATION**

CORROSIVE (C, R34 OR R35)	NO	D
IRRITATING TO SKIN (XI, R38)	NO	D
IRRITATING TO EYES (XI, R36)	NO	D
RISK OF SERIOUS DAMAGE TO EYES (XI, R41)	NO	D
IRRITATING TO RESPIRATORY SYSTEM (XI, R37)	NO	D
MAY CAUSE SENSITISATION BY INHALATION (XN, R42)	NO	D
MAY CAUSE SENSITISATION BY SKIN CONTACT (XI, R43)	NO	D
MAY CAUSE CANCER (T, R45)	NO	D
MAY CAUSE CANCER BY INHALATION (T, R49)	NO	D
POSSIBLE RISK OF IRREVERSIBLE EFFECTS (XN, R40)	NO	D

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