

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 13.08.2018

Version 15.3

SECTION 1. Identification of the substance/mixture and of the company/undertaking

1.1 Product identifier

Catalogue No.	804918
Product name	Potassium tert-butyrate for synthesis
REACH Registration Number	01-2119971575-26-XXXX
CAS-No.	865-47-4

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses	Chemical for synthesis
	In compliance with the conditions described in the annex to this safety data sheet.

1.3 Details of the supplier of the safety data sheet

Company	Merck KGaA * 64271 Darmstadt * Germany * Phone:+49 6151 72-0
Responsible Department	LS-QHC * e-mail: prodsafe@merckgroup.com

1.4 Emergency telephone number	Please contact the regional company representation in your country.
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SECTION 2. Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Flammable solid, Category 1, H228

Skin corrosion, Category 1A, H314

For the full text of the H-Statements mentioned in this Section, see Section 16.

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Catalogue No.

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Product name

Potassium tert-butyrate for synthesis

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

Danger

Hazard statements

H228 Flammable solid.

H314 Causes severe skin burns and eye damage.

EUH014 Reacts violently with water.

Precautionary statements

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

Response

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

P370 + P378 In case of fire: Use powder for extinction.

Reduced labelling (≤125 ml)

Hazard pictograms



Signal word

Danger

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Product name Potassium tert-butyrate for synthesis

Hazard statements

H314 Causes severe skin burns and eye damage.
EUH014 Reacts violently with water.

Precautionary statements

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.
P370 + P378 In case of fire: Use powder for extinction.

CAS-No. 865-47-4

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	(CH ₃) ₃ COK	C ₄ H ₉ KO (Hill)
EC-No.	212-740-3	
Molar mass	112,21 g/mol	

Hazardous components (REGULATION (EC) No 1272/2008)

Chemical name (Concentration)

CAS-No.	Registration number	Classification
potassium tert-butanolate (<= 100 %)		

Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

865-47-4	01-2119971575-26-	
	XXXX	Flammable solid, Category 1, H228 Skin corrosion, Category 1A, H314

For the full text of the H-Statements mentioned in this Section, see Section 16.

3.2 Mixture

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Not applicable

SECTION 4. First aid measures

4.1 Description of first aid measures

General advice

First aider needs to protect himself.

After inhalation: fresh air. Call in physician.

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower. Call a physician immediately.

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

4.2 Most important symptoms and effects, both acute and delayed

Irritation and corrosion, Cough, Shortness of breath

Risk of blindness!

4.3 Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂), Dry powder, Sand, Cement

Unsuitable extinguishing media

Water, Foam

5.2 Special hazards arising from the substance or mixture

Combustible.

Risk of dust explosion.

Self-ignition possible due to air moisture.

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Development of hazardous combustion gases or vapours possible in the event of fire.

May not get in touch with:

Water

5.3 Advice for firefighters

Special protective equipment for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

Further information

Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders:

Protective equipment see section 8.

6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 Reference to other sections

Indications about waste treatment see section 13.

SECTION 7. Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Observe label precautions.

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Keep workplace dry. Do not allow product to come into contact with water.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

7.2 Conditions for safe storage, including any incompatibilities

Requirements for storage areas and containers

No metal or light-weight-metal containers.

Storage conditions

Protective gas: Argon.

Tightly closed. Dry. Keep away from heat and sources of ignition.

Recommended storage temperature see product label.

7.3 Specific end use(s)

See exposure scenario in the Annex to this MSDS.

SECTION 8. Exposure controls/personal protection

8.1 Control parameters

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Derived No Effect Level (DNEL)

Worker DNEL, longterm	Systemic effects	inhalation	1 mg/m ³
Worker DNEL, acute	Systemic effects	inhalation	1 mg/m ³
Worker DNEL, longterm	Local effects	inhalation	1 mg/m ³
Worker DNEL, acute	Local effects	inhalation	1 mg/m ³

Predicted No Effect Concentration (PNEC)

PNEC Fresh water	0,11 mg/l
PNEC Marine water	0,011 mg/l
PNEC Aquatic intermittent release	1,1 mg/l
PNEC Sediment	0,419 mg/kg
PNEC Marine sediment	0,0419 mg/kg
PNEC Sewage treatment plant	10 mg/l
PNEC Soil	0,0192 mg/kg

8.2 Exposure controls

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

Eye/face protection

Tightly fitting safety goggles

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Hand protection

full contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 741 Dermatril® L (full contact), KCL 741 Dermatril® L (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

This recommendation applies only to the product stated in the safety data sheet(>,<)> supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Other protective equipment

Flame retardant antistatic protective clothing.

Respiratory protection

required when dusts are generated.

Recommended Filter type: Filter P 2 (acc. to DIN 3181) for solid and liquid particles of harmful substances

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Environmental exposure controls

Do not let product enter drains.

Risk of explosion.

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SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	powder
Colour	light yellow
Odour	odourless
Odour Threshold	Not applicable
pH	ca. 13 at 5 g/l 20 °C Hydrolysis
Melting point	256 - 258 °C
Boiling point	No information available.
Flash point	Not applicable
Evaporation rate	No information available.
Flammability (solid, gas)	The substance or mixture is a flammable solid with the category 1. Flammability (solids) NF T 20-042
Lower explosion limit	No information available.
Upper explosion limit	No information available.

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Vapour pressure	0,02 hPa at 20 °C Method: OECD Test Guideline 104
Relative vapour density	No information available.
Density	1,19 g/cm ³ at 20 °C Method: OECD Test Guideline 109
Relative density	No information available.
Water solubility	at 20 °C Hydrolysis, (rigorous decomposition)
Partition coefficient: n-octanol/water	Not applicable
Auto-ignition temperature	No information available.
Decomposition temperature	300 °C Method: OECD Test Guideline 113
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Oxidizing properties	none

9.2 Other data

Sublimation point	220 °C at 1,33 hPa
Ignition temperature	483 °C

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Product name	Potassium tert-butyrate for synthesis

Bulk density	ca.500 kg/m ³
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SECTION 10. Stability and reactivity

10.1 Reactivity

Self-ignition possible due to air moisture.

Risk of dust explosion.

Reacts violently with water.

Self-heating in large quantities; may catch fire.

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

10.2 Chemical stability

sensitive to moisture

Sensitive to air.

In case of decomposition in closed containers and tubes risk of bursting due to buildup of overpressure.

sensitive to moisture

10.3 Possibility of hazardous reactions

Risk of ignition or formation of inflammable gases or vapours with:

Water, Acetone, Alcohols, Chloroform, dichloromethane, acetic acid, ethanol, Esters, Methanol, sulphuric acid, halogens, acids, DIETHYL SULPHATE

Exothermic reaction with:

Halogenated hydrocarbon

10.4 Conditions to avoid

Moisture.

10.5 Incompatible materials

Light metals, light metal alloys, Metals

10.6 Hazardous decomposition products

no information available

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SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the oesophagus and the stomach.

Acute inhalation toxicity

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract

Acute dermal toxicity

This information is not available.

Skin irritation

Rabbit

Result: Causes severe burns.

OECD Test Guideline 404

Causes severe burns.

Eye irritation

Causes serious eye damage.

Risk of blindness!

Sensitisation

This information is not available.

Germ cell mutagenicity

This information is not available.

Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

Teratogenicity

This information is not available.

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Product name	Potassium tert-butyrate for synthesis

Specific target organ toxicity - single exposure

This information is not available.

Specific target organ toxicity - repeated exposure

This information is not available.

Aspiration hazard

This information is not available.

11.2 Further information

Handle in accordance with good industrial hygiene and safety practice.

Other dangerous properties can not be excluded.

SECTION 12. Ecological information

12.1 Toxicity

No information available.

12.2 Persistence and degradability

Biodegradability

decomposes

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

Not applicable

12.4 Mobility in soil

No information available.

12.5 Results of PBT and vPvB assessment

Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

12.6 Other adverse effects

Additional ecological information

Product reacts with water. Harmful effect due to pH shift. Discharge into the environment must be avoided.

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Product name	Potassium tert-butylate for synthesis

SECTION 13. Disposal considerations

Waste treatment methods

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14. Transport information

Land transport (ADR/RID)

14.1 UN number	UN 2921
14.2 Proper shipping name	CORROSIVE SOLID, FLAMMABLE, N.O.S. (POTASSIUM-TERT-BUTYLATE)
14.3 Class	8 (4.1)
14.4 Packing group	I
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
Tunnel restriction code	E

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 UN number	UN 2921
14.2 Proper shipping name	CORROSIVE SOLID, FLAMMABLE, N.O.S. (POTASSIUM-TERT-BUTYLATE)
14.3 Class	8 (4.1)
14.4 Packing group	I
14.5 Environmentally hazardous	--
14.6 Special precautions for user	no

Sea transport (IMDG)

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Catalogue No.	804918
Product name	Potassium tert-butylate for synthesis

14.1 UN number	UN 2921
14.2 Proper shipping name	CORROSIVE SOLID, FLAMMABLE, N.O.S. (POTASSIUM-TERT-BUTYLATE)
14.3 Class	8 (4.1)
14.4 Packing group	I
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
EmS	F-A S-G
Segregation Group	0018 Alkalis
14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code	
Not relevant	

SECTION 15. Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

EU regulations

Major Accident Hazard	SEVESO III
Legislation	OTHER HAZARDS O1 Quantity 1: 100 t Quantity 2: 500 t

Occupational restrictions	Take note of Dir 94/33/EC on the protection of young people at work.
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Regulation (EC) No 1005/2009 on substances that deplete the ozone layer	not regulated
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Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC	not regulated
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Substances of very high concern (SVHC)

This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of $\geq 0.1\%$ (w/w).

National legislation

Storage class 4.1B

Dust explosion class St3

15.2 Chemical safety assessment

A Chemical Safety Assessment has been carried out according to regulation (EC) No. 1907/2006 (REACH) for this substance.

SECTION 16. Other information

Full text of H-Statements referred to under sections 2 and 3.

H228 Flammable solid.

H314 Causes severe skin burns and eye damage.

Training advice

Provide adequate information, instruction and training for operators.

Labelling

Hazard pictograms



Signal word

Danger

Hazard statements

H228 Flammable solid.

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Catalogue No.	804918
Product name	Potassium tert-butyrate for synthesis

H314 Causes severe skin burns and eye damage.

EUH014 Reacts violently with water.

Precautionary statements

Prevention

P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.

P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

Response

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

P370 + P378 In case of fire: Use powder for extinction.

Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Regional representation

This information is given on the authorised Safety Data Sheet for your country.

The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.

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Product name	Potassium tert-butyrate for synthesis

EXPOSURE SCENARIO 1 (Industrial use)

1. Industrial use Chemical for synthesis)

Sectors of end-use

<i>SU 3</i>	Industrial uses: Uses of substances as such or in preparations at industrial sites
<i>SU9</i>	Manufacture of fine chemicals
<i>SU 10</i>	Formulation [mixing] of preparations and/ or re-packaging (excluding alloys)

Chemical product category

<i>PC19</i>	Intermediate
<i>PC21</i>	Laboratory chemicals

Process categories

<i>PROC1</i>	Use in closed process, no likelihood of exposure
<i>PROC2</i>	Use in closed, continuous process with occasional controlled exposure
<i>PROC3</i>	Use in closed batch process (synthesis or formulation)
<i>PROC4</i>	Use in batch and other process (synthesis) where opportunity for exposure arises
<i>PROC5</i>	Mixing or blending in batch processes for formulation of preparations and articles (multistage and/ or significant contact)
<i>PROC8a</i>	Transfer of substance or preparation (charging/ discharging) from/ to vessels/ large containers at non-dedicated facilities
<i>PROC8b</i>	Transfer of substance or preparation (charging/ discharging) from/ to vessels/ large containers at dedicated facilities
<i>PROC9</i>	Transfer of substance or preparation into small containers (dedicated filling line, including weighing)
<i>PROC15</i>	Use as laboratory reagent

Environmental Release Categories

<i>ERC1</i>	Manufacture of substances
<i>ERC2</i>	Formulation of preparations
<i>ERC4</i>	Industrial use of processing aids in processes and products, not becoming part of articles
<i>ERC6a</i>	Industrial use resulting in manufacture of another substance (use of intermediates)
<i>ERC6b</i>	Industrial use of reactive processing aids

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2. Contributing scenarios: Operational conditions and risk management measures

2.1 Contributing scenario controlling worker exposure for: PROC1, PROC2, PROC3, PROC4, PROC5, PROC8a, PROC8b, PROC9, PROC15

Product characteristics

Concentration of the Substance in Mixture/Article	Covers the percentage of the substance in the product up to 100 %.
Physical Form (at time of use)	Very low volatile liquid
Process Temperature	< 250 °C

Frequency and duration of use

Frequency of use	8 hours/day
Frequency of use	5 days/week

Other operational conditions affecting workers exposure

Outdoor / Indoor	Indoor without local exhaust ventilation (LEV)
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Organisational measures to prevent /limit releases, dispersion and exposure

Covers daily exposures up to 8 hours.

Conditions and measures related to personal protection, hygiene and health evaluation

Wear chemically resistant gloves (tested to EN374) in combination with specific activity training. Tightly fitting safety goggles

Additional good practice advice beyond the REACH Chemical Safety Assessment

Additional good practice advice	Wear suitable coveralls to prevent exposure to the skin.
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3. Exposure estimation and reference to its source

Environment

A chemical safety assessment was performed according REACH Article 14(3), Annex I, sections 3 (Environmental Hazard Assessment) and 4 (PBT/vPvB Assessment). As no hazard was identified, an exposure assessment and risk characterisation is not necessary (REACH Annex I section 5.0).

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Product name Potassium tert-butylate for synthesis

Workers

CS	Use descriptor	Exposure duration, route, effect	RCR	Exposure Assessment Method
2.1	PROC1	longterm, inhalative, systemic	0,047	ECETOC TRA
2.1	PROC2	longterm, inhalative, systemic	0,47	ECETOC TRA
2.1	PROC3	longterm, inhalative, systemic	0,47	ECETOC TRA
2.1	PROC4	longterm, inhalative, systemic	0,47	ECETOC TRA
2.1	PROC5	longterm, inhalative, systemic	0,47	ECETOC TRA
2.1	PROC8a	longterm, inhalative, systemic	0,47	ECETOC TRA
2.1	PROC8b	longterm, inhalative, systemic	0,47	ECETOC TRA
2.1	PROC9	longterm, inhalative, systemic	0,47	ECETOC TRA
2.1	PROC15	longterm, inhalative, systemic	0,47	ECETOC TRA

The default parameters and -efficiencies of the applied exposure assessment model were used for the calculation (unless stated differently).

For (other) acute and local effects risk management measures are based on qualitative risk characterisation.

4. Guidance to Downstream User to evaluate whether he works inside the boundaries set by the Exposure Scenario

Please refer to the following documents: ECHA Guidance on information requirements and chemical safety assessment Chapter R.12: Use descriptor system; ECHA Guidance for downstream users; ECHA Guidance on information requirements and chemical safety assessment Part D: Exposure Scenario Building, Part E: Risk Characterisation and Part G: Extending the SDS; VCI/Cefic REACH Practical Guides on Exposure Assessment and Communications in the Supply Chain; CEFIC Guidance Specific Environmental Release Categories (SPERCs).

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For scaling of worker exposure assessments performed with ECETOC TRA, please consult the Merck tool SciDeEx® at www.merckmillipore.com/scideex.

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EXPOSURE SCENARIO 2 (Professional use)

1. Professional use Chemical for synthesis)

Sectors of end-use

SU 22 Professional uses: Public domain (administration, education, entertainment, services, craftsmen)

Chemical product category

PC21 Laboratory chemicals

Process categories

PROC15 Use as laboratory reagent

Environmental Release Categories

ERC2 Formulation of preparations

ERC6a Industrial use resulting in manufacture of another substance (use of intermediates)

ERC6b Industrial use of reactive processing aids

2. Contributing scenarios: Operational conditions and risk management measures

2.1 Contributing scenario controlling worker exposure for: PROC15

Product characteristics

Concentration of the Substance in Mixture/Article	Covers the percentage of the substance in the product up to 100 %.
Physical Form (at time of use)	Very low volatile liquid
Process Temperature	< 250 °C

Frequency and duration of use

Frequency of use	8 hours/day
Frequency of use	5 days/week

Other operational conditions affecting workers exposure

Outdoor / Indoor	Indoor without local exhaust ventilation (LEV)
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Organisational measures to prevent /limit releases, dispersion and exposure

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Product name Potassium tert-butyrate for synthesis

Covers daily exposures up to 8 hours.

Conditions and measures related to personal protection, hygiene and health evaluation

Wear chemically resistant gloves (tested to EN374) in combination with specific activity training. Tightly fitting safety goggles

Additional good practice advice beyond the REACH Chemical Safety Assessment

Additional good practice advice Wear suitable coveralls to prevent exposure to the skin.

3. Exposure estimation and reference to its source

Environment

A chemical safety assessment was performed according REACH Article 14(3), Annex I, sections 3 (Environmental Hazard Assessment) and 4 (PBT/vPvB Assessment). As no hazard was identified, an exposure assessment and risk characterisation is not necessary (REACH Annex I section 5.0).

Workers

CS	Use descriptor	Exposure duration, route, effect	RCR	Exposure Assessment Method
2.1	PROC15	longterm, inhalative, systemic	0,47	ECETOC TRA

The default parameters and -efficiencies of the applied exposure assessment model were used for the calculation (unless stated differently).

For (other) acute and local effects risk management measures are based on qualitative risk characterisation.

4. Guidance to Downstream User to evaluate whether he works inside the boundaries set by the Exposure Scenario

Please refer to the following documents: ECHA Guidance on information requirements and chemical safety assessment Chapter R.12: Use descriptor system; ECHA Guidance for downstream users; ECHA Guidance on information requirements and chemical safety assessment Part D: Exposure Scenario Building, Part E: Risk Characterisation and Part G: Extending the SDS; VCI/Cefic REACH Practical Guides on Exposure Assessment and Communications in the Supply Chain; CEFIC Guidance Specific Environmental Release Categories (SPERCs).

For scaling of worker exposure assessments performed with ECETOC TRA, please consult the Merck

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tool SciDeEx® at www.merckmillipore.com/scideex.