

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1. Product identifier**

Product form : Substance
Name : tert-butyl (5-bromo-3-(3-(4-(((tert-butoxycarbonyl)(methyl)amino)methyl)phenyl)isoxazol-5-yl)pyrazin-2-yl)(tert-butoxycarbonyl)carbamate
CAS-No. : 1402390-42-4
Formula : $C_{30}H_{38}BrN_5O_7$
Synonyms : MSC2621052, Compound E

1.2. Relevant identified uses of the substance or mixture and uses advised against**1.2.1. Relevant identified uses**

Main use category : Industrial use
Industrial/Professional use spec : For professional use only
Use of the substance/mixture : Intermediates

1.2.2. Uses advised against

No additional information available

1.3. Details of the supplier of the safety data sheet

SK Biotek Ireland, Ltd.
Watery Lane, Swords
Dublin - Ireland
T +353 1813 9456
SDS-Ireland@SK.com - <https://skbiotek.ie/>

1.4. Emergency telephone number

Country	Organisation/Company	Address	Emergency number	Comment
Ireland	National Poisons Information Centre Beaumont Hospital	PO Box 1297 Beaumont Road 9 Dublin	+353 1 809 2566 (Healthcare professionals- 24/7) +353 1 809 2166 (public, 8am - 10pm, 7/7)	

SECTION 2: Hazards identification**2.1. Classification of the substance or mixture**

Classification according to Regulation (EC) No. 1272/2008 [CLP]

Not classified

Adverse physicochemical, human health and environmental effects

No additional information available

2.2. Label elements

Labelling according to Regulation (EC) No. 1272/2008 [CLP]

No labelling applicable

2.3. Other hazards

PBT: not yet assessed

vPvB: not yet assessed

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according to Regulation (EU) 2020/878

SECTION 3: Composition/information on ingredients

3.1. Substances

Name	Product identifier	Conc.	Classification according to Regulation (EC) No. 1272/2008 [CLP]
tert-butyl (5-bromo-3-(3-(4-(((tert-butoxycarbonyl)(methyl)amino)methyl)phenyl)isoxazol-5-yl)pyrazin-2-yl)(tert-butoxycarbonyl)carbamate	(CAS-No.) 1402390-42-4	> 99	Not classified

3.2. Mixtures

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general	: If you feel unwell, seek medical advice (show the label where possible).
First-aid measures after inhalation	: Remove person to fresh air and keep comfortable for breathing. If experiencing respiratory symptoms: Call a poison center or a doctor.
First-aid measures after skin contact	: Wash skin thoroughly with mild soap and water. Get medical attention if symptoms occur.
First-aid measures after eye contact	: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get medical attention if symptoms occur.
First-aid measures after ingestion	: Never give anything by mouth to an unconscious person. Do not induce vomiting. Rinse mouth. In case of doubt or persistent symptoms, consult always a physician.

4.2. Most important symptoms and effects, both acute and delayed

Symptoms/effects after inhalation	: Not expected to present a significant hazard under anticipated conditions of normal use. Dust of the product, if present, may cause respiratory irritation after an excessive inhalation exposure.
Symptoms/effects after skin contact	: Dust may cause irritation in skin folds or by contact in combination with tight clothing.
Symptoms/effects after eye contact	: Not expected to present a significant eye contact hazard under anticipated conditions of normal use. Dust from the product, if present, may cause a mechanical eye irritation, redness and lacrimation.
Symptoms/effects after ingestion	: Ingestion may cause nausea, vomiting and diarrhea.

4.3. Indication of any immediate medical attention and special treatment needed

Treat symptomatically.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media	: Dry chemical, CO ₂ , or water spray or regular foam. Use extinguishing agent suitable for surrounding fire.
Unsuitable extinguishing media	: Do not use a heavy water stream.

5.2. Special hazards arising from the substance or mixture

Fire hazard	: Burning produces irritating, toxic and noxious fumes. Do not breathe fumes from fires or vapours from decomposition.
Hazardous decomposition products in case of fire	: Toxic fumes may be released. Thermal decomposition generates : Carbon dioxide. Carbon monoxide. Nitrogen oxides.

5.3. Advice for firefighters

Firefighting instructions	: Move containers from fire area if it can be done without personal risk. Exercise caution when fighting any chemical fire. Fight fire with normal precautions from a reasonable distance. Evacuate the danger area.
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Protection during firefighting : Do not enter fire area without proper protective equipment, including respiratory protection. Wear fire/flame resistant/retardant clothing. Collect firefighting water.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures : Avoid contact with skin and eyes. Prevent from entering sewers, basements and workpits, or any place where its accumulation can be dangerous.

6.1.1. For non-emergency personnel

Protective equipment : Wear recommended personal protective equipment.
Emergency procedures : Ventilate spillage area. Evacuate unnecessary personnel. Do not get in eyes, on skin, or on clothing. Do not touch or walk on the spilled product. No action shall be taken without appropriate training or involving any personal risk. Avoid creating or spreading dust.

6.1.2. For emergency responders

Protective equipment : Do not attempt to take action without suitable protective equipment. For further information refer to section 8: "Exposure controls/personal protection".
Emergency procedures : Ventilate area. Avoid creating or spreading dust. Avoid breathing dust.

6.2. Environmental precautions

Do not allow product to spread into the environment. Prevent entry to sewers and public waters. Notify authorities if product enters sewers or public waters.

6.3. Methods and material for containment and cleaning up

For containment : Contain any spills with dikes or absorbents to prevent migration and entry into sewers or streams.
Methods for cleaning up : Take up mechanically (sweeping, shovelling) and collect in suitable container for disposal. Minimise generation of dust. Ventilate spillage area.
Other information : Dispose of materials or solid residues at an authorized site.

6.4. Reference to other sections

For further information refer to section 13. For further information refer to section 8: "Exposure controls/personal protection".

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Do not handle until all safety precautions have been read and understood. Provide adequate ventilation to minimize dust and/or vapour concentrations. Take all necessary technical measures to avoid or minimize the release of the product on the workplace. Use personal protective equipment as required. Avoid contact with skin and eyes.
Hygiene measures : Handle in accordance with good industrial hygiene and safety procedures. Do not eat, drink or smoke when using this product. Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Contaminated work clothing should not be allowed out of the workplace.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions : Keep away from food, drink and animal feedingstuffs. Store in a well-ventilated place. Store in a dry place. Store in original container.
Incompatible products : Oxidizing agent. Strong bases. Protect from moisture.
Incompatible materials : Heat sources. Light sources.
Storage temperature : room temperature
Packaging materials : Aluminium.

7.3. Specific end use(s)

No additional information available

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SECTION 8: Exposure controls/personal protection

8.1. Control parameters

8.1.1 National occupational exposure and biological limit values

No additional information available

8.1.2. Recommended monitoring procedures

No additional information available

8.1.3. Air contaminants formed

No additional information available

8.1.4. DNEL and PNEC

No additional information available

8.1.5. Control banding

Control banding : SK Biotek Exposure Control Band (Band 4) = 1-10 ug/m3

8.2. Exposure controls

8.2.1. Appropriate engineering controls

Appropriate engineering controls:

Use engineering controls to keep exposures below the OEL or DNEL. Provide local exhaust ventilation.

8.2.2. Personal protection equipment

8.2.2.1. Eye and face protection

Eye protection:

In case of dust production: protective goggles

8.2.2.2. Skin protection

Skin and body protection:

Skin protection appropriate to the conditions of use should be provided

Hand protection:

Chemical resistant gloves (according to European standard EN 374 or equivalent). Please follow the instructions related to the permeability and the penetration time provided by the manufacturer

Other skin protection

Materials for protective clothing:

PPE compliant to the recommended EN/ISO standards should be selected.

8.2.2.3. Respiratory protection

Respiratory protection:

No respiratory protection needed under normal use conditions. Where excessive vapour, mist, or dust may result, use approved respiratory protection equipment

8.2.2.4. Thermal hazards

No additional information available

8.2.3. Environmental exposure controls

Environmental exposure controls:

Avoid release to the environment.

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SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Solid
Appearance	: Powder.
Molecular mass	: 660.56 g/mol
Colour	: Yellow.
Odour	: No data available
Odour threshold	: No data available
pH	: No data available
Relative evaporation rate (butylacetate=1)	: No data available
Melting point	: No data available
Freezing point	: Not applicable
Boiling point	: Not applicable
Flash point	: Not applicable
Auto-ignition temperature	: Not applicable
Decomposition temperature	: No data available
Flammability (solid, gas)	: No data available
Vapour pressure	: Not applicable
Relative vapour density at 20 °C	: Not applicable
Relative density	: No data available
Solubility	: No data available
Partition coefficient n-octanol/water (Log Pow)	: No data available
Viscosity, kinematic	: Not applicable
Viscosity, dynamic	: Not applicable
Explosive properties	: No data available
Oxidising properties	: No data available
Explosive limits	: Not applicable

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

The product is non-reactive under normal conditions of use, storage and transport.

10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

No dangerous reactions known under normal conditions of use. Hazardous polymerisation: Will not occur.

10.4. Conditions to avoid

Overheating. Moisture.

10.5. Incompatible materials

Oxidizing agent. Strong bases.

10.6. Hazardous decomposition products

Under normal conditions of storage and use, hazardous decomposition products should not be produced.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity (oral)	: Not classified (Based on available data, the classification criteria are not met)
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Acute toxicity (dermal)	: Not classified (Based on available data, the classification criteria are not met)
Acute toxicity (inhalation)	: Not classified (Based on available data, the classification criteria are not met)
Skin corrosion/irritation	: Not classified (Based on available data, the classification criteria are not met)
Serious eye damage/irritation	: Not classified (Based on available data, the classification criteria are not met)
Respiratory or skin sensitisation	: Not classified (Based on available data, the classification criteria are not met)
Germ cell mutagenicity	: Not classified (Based on available data, the classification criteria are not met)
Carcinogenicity	: Not classified (Based on available data, the classification criteria are not met)
Reproductive toxicity	: Not classified (Based on available data, the classification criteria are not met)
STOT-single exposure	: Not classified (Based on available data, the classification criteria are not met)
STOT-repeated exposure	: Not classified (Based on available data, the classification criteria are not met)
Aspiration hazard	: Not classified (Based on available data, the classification criteria are not met)

tert-butyl (5-bromo-3-(3-(4-(((tert-butoxycarbonyl)(methyl)amino)methyl)phenyl)isoxazol-5-yl)pyrazin-2-yl)(tert-butoxycarbonyl)carbamate (1402390-42-4)

Viscosity, kinematic	Not applicable
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SECTION 12: Ecological information

12.1. Toxicity

Hazardous to the aquatic environment, short-term (acute)	: Not classified (Lack of data)
Hazardous to the aquatic environment, long-term (chronic)	: Not classified (Lack of data)
Not rapidly degradable	

12.2. Persistence and degradability

tert-butyl (5-bromo-3-(3-(4-(((tert-butoxycarbonyl)(methyl)amino)methyl)phenyl)isoxazol-5-yl)pyrazin-2-yl)(tert-butoxycarbonyl)carbamate (1402390-42-4)

Persistence and degradability	Biodegradability in water: no data available.
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12.3. Bioaccumulative potential

tert-butyl (5-bromo-3-(3-(4-(((tert-butoxycarbonyl)(methyl)amino)methyl)phenyl)isoxazol-5-yl)pyrazin-2-yl)(tert-butoxycarbonyl)carbamate (1402390-42-4)

Bioaccumulative potential	No bioaccumulation data available.
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12.4. Mobility in soil

tert-butyl (5-bromo-3-(3-(4-(((tert-butoxycarbonyl)(methyl)amino)methyl)phenyl)isoxazol-5-yl)pyrazin-2-yl)(tert-butoxycarbonyl)carbamate (1402390-42-4)

Ecology - soil	Not established.
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12.5. Results of PBT and vPvB assessment

tert-butyl (5-bromo-3-(3-(4-(((tert-butoxycarbonyl)(methyl)amino)methyl)phenyl)isoxazol-5-yl)pyrazin-2-yl)(tert-butoxycarbonyl)carbamate (1402390-42-4)

PBT: not yet assessed

vPvB: not yet assessed

12.6. Other adverse effects

Other adverse effects	: No other effects known.
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SECTION 13: Disposal considerations

13.1. Waste treatment methods

- Waste treatment methods : Dispose of contents/container in accordance with licensed collector's sorting instructions. Disposal must be carried out using appropriate EWC code.
- Product/Packaging disposal recommendations : Completely empty the packaging prior to decontamination. Dispose in a safe manner in accordance with local/national regulations. Do not dispose of the packaging without first carrying out the necessary cleaning.

SECTION 14: Transport information

In accordance with ADR / IMDG / IATA / ADN / RID

ADR	IMDG	IATA	ADN	RID
14.1. UN number				
Not applicable	Not applicable	Not applicable	Not applicable	Not applicable
14.2. UN proper shipping name				
Not applicable	Not applicable	Not applicable	Not applicable	Not applicable
14.3. Transport hazard class(es)				
Not applicable	Not applicable	Not applicable	Not applicable	Not applicable
14.4. Packing group				
Not applicable	Not applicable	Not applicable	Not applicable	Not applicable
14.5. Environmental hazards				
Not applicable	Not applicable	Not applicable	Not applicable	Not applicable
No supplementary information available				

14.6. Special precautions for user

Overland transport

Not applicable

Transport by sea

Not applicable

Air transport

Not applicable

Inland waterway transport

Not applicable

Rail transport

Not applicable

14.7. Transport in bulk according to Annex II of Marpol and the IBC Code

Not applicable

SECTION 15: Regulatory information

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

15.1.1. EU-Regulations

No REACH Annex XVII restrictions

tert-butyl (5-bromo-3-(3-(4-(((tert-butoxycarbonyl)(methyl)amino)methyl)phenyl)isoxazol-5-yl)pyrazin-2-yl)(tert-butoxycarbonyl)carbamate is not on the REACH Candidate List

tert-butyl (5-bromo-3-(3-(4-(((tert-butoxycarbonyl)(methyl)amino)methyl)phenyl)isoxazol-5-yl)pyrazin-2-yl)(tert-butoxycarbonyl)carbamate is not on the REACH Annex XIV List

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tert-butyl (5-bromo-3-(3-(4-(((tert-butoxycarbonyl)(methyl)amino)methyl)phenyl)isoxazol-5-yl)pyrazin-2-yl)(tert-butoxycarbonyl)carbamate is not subject to Regulation (EU) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of hazardous chemicals.

tert-butyl (5-bromo-3-(3-(4-(((tert-butoxycarbonyl)(methyl)amino)methyl)phenyl)isoxazol-5-yl)pyrazin-2-yl)(tert-butoxycarbonyl)carbamate is not subject to Regulation (EU) No 2019/1021 of the European Parliament and of the Council of 20 June 2019 on persistent organic pollutants

15.1.2. National regulations

No additional information available

15.2. Chemical safety assessment

No chemical safety assessment has been carried out

SECTION 16: Other information

Abbreviations and acronyms:	
ADN	European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways
ADR	European Agreement concerning the International Carriage of Dangerous Goods by Road
ATE	Acute Toxicity Estimate
BLV	Biological limit value
CAS-No.	Chemical Abstract Service number
CLP	Classification Labelling Packaging Regulation; Regulation (EC) No 1272/2008
DMEL	Derived Minimal Effect level
DNEL	Derived-No Effect Level
EC50	Median effective concentration
EC-No.	European Community number
EN	European Standard
IATA	International Air Transport Association
IMDG	International Maritime Dangerous Goods
LC50	Median lethal concentration
LD50	Median lethal dose
LOAEL	Lowest Observed Adverse Effect Level
NOAEC	No-Observed Adverse Effect Concentration
NOAEL	No-Observed Adverse Effect Level
NOEC	No-Observed Effect Concentration
OEL	Occupational Exposure Limit
PBT	Persistent Bioaccumulative Toxic
PNEC	Predicted No-Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals Regulation (EC) No 1907/2006
RID	Regulations concerning the International Carriage of Dangerous Goods by Rail
SDS	Safety Data Sheet
vPvB	Very Persistent and Very Bioaccumulative
WGK	Water Hazard Class

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Data sources : REGULATION (EC) No 1272/2008 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006. Quantitative structure-activity relationship (QSAR).

Training advice : Training staff on good practice.

Safety Data Sheet (SDS), EU_orange

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.