

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

Product form	: Substance
Trade name	: SITAGLIPTIN HYDROCHLORIDE MONOHYDRATE
Chemical name	: 1,2,4-Triazolo[4,3-a]pyrazine, 7-[(3R)-3-amino-1-oxo-4-(2,4,5-trifluorophenyl)butyl]-5,6,7,8-tetrahydro-3-(trifluoromethyl)-, monohydrochloride, monohydrate (9CI)
IUPAC name	: (3R)-3-amino-1-[3-(trifluoromethyl)-6,8-dihydro-5H-[1,2,4]triazolo[4,3-a]pyrazin-7-yl]-4-(2,4,5-trifluorophenyl)butan-1-one;hydrate;hydrochloride
CAS-No.	: 862156-92-1
Product code	: 94580 / 94590
Formula	: C16H15F6N5O.HCl.H2O
Product group	: Active Ingredient for Medicinal/Pharmaceutical Use
Other means of identification	: SMILES: N[C@@H](CC(=O)N1CCN2C(C1)=NN=C2C(F)(F)F)CC1=CC(F)=C(F)C=C1F.Cl.H2O ; c1c(c(cc1F)F)C[C@H](CC(=O)N2CCn3c(nnc3C(F)(F)F)C2)N.Cl.H2O

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,API
Industrial/Professional use spec	: Industrial For professional use only
Function or use category	: Pharmaceuticals

1.2.2. Uses advised against

No additional information available

1.3. Details of the supplier of the safety data sheet**Head office**

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Manufacturer

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B-7860 Lessines
Belgium
T + 32 68 33 49 13

1.4. Emergency telephone number

Emergency number	: +34 93 586 05 20 (9:00 - 17:00)
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SECTION 2: Hazards identification**2.1. Classification of the substance or mixture****Classification according to Regulation (EC) No. 1272/2008 [CLP]**

Skin corrosion/irritation, Category 2	H315
Serious eye damage/eye irritation, Category 2	H319
Specific target organ toxicity – Single exposure, Category 3, Respiratory tract irritation	H335

Full text of H- and EUH-statements: see section 16

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according to the REACH Regulation (EC) 1907/2006 amended by Regulation (EU) 2020/878

Adverse physicochemical, human health and environmental effects

Causes skin and eye irritation. May cause respiratory irritation.

2.2. Label elements

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

Hazard pictograms (CLP)



GHS07

Signal word (CLP)

: Warning

Hazard statements (CLP)

: H315 - Causes skin irritation.

H319 - Causes serious eye irritation.

H335 - May cause respiratory irritation.

Precautionary statements (CLP)

: P261 - Avoid breathing dust.

P264 - Wash hands, forearms and face thoroughly after handling.

P271 - Use only outdoors or in a well-ventilated area.

P280 - Wear protective gloves, face protection, eye protection.

P302+P352 - IF ON SKIN: Wash with plenty of water.

P304+P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing.

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

P332+P313 - If skin irritation occurs: Get medical advice/attention.

P337+P313 - If eye irritation persists: Get medical advice/attention.

P362+P364 - Take off contaminated clothing and wash it before reuse.

P501 - Dispose of contents and container to hazardous or special waste collection point, in accordance with local, regional, national and/or international regulation.

2.3. Other hazards

Other hazards which do not result in classification : Dust may form explosive mixture in air.

SECTION 3: Composition/information on ingredients

3.1. Substances

Substance type : Mono-constituent

Name	Product identifier	%
SITAGLIPTIN HYDROCHLORIDE MONOHYDRATE	CAS-No.: 862156-92-1	100

3.2. Mixtures

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general	: Never give anything by mouth to an unconscious person. 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. Call a POISON CENTER/doctor if you feel unwell.
First-aid measures after skin contact	: Remove affected clothing and wash all exposed skin area with mild soap and water, followed by warm water rinse. If skin irritation occurs: Get medical advice/attention.
First-aid measures after eye contact	: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice/attention.
First-aid measures after ingestion	: Rinse mouth. Do NOT induce vomiting. Obtain emergency medical attention.

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

Symptoms/effects after inhalation	: May cause respiratory irritation.
Symptoms/effects after skin contact	: Causes skin irritation.
Symptoms/effects after eye contact	: Causes serious eye irritation.

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

No additional information available

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media	: Foam. Dry powder. Carbon dioxide. Water spray. Sand.
Unsuitable extinguishing media	: Do not use a heavy water stream.

5.2. Special hazards arising from the substance or mixture

Explosion hazard	: Avoid raising powdered material due to explosion hazard.
Hazardous decomposition products in case of fire	: fume. Carbon monoxide. Carbon dioxide. Nitrogen oxides.

5.3. Advice for firefighters

Precautionary measures fire	: Keep away from combustible materials. Minimize generation of dust which may be combustible.
Firefighting instructions	: Use water spray or fog for cooling exposed containers. Exercise caution when fighting any chemical fire. Prevent fire fighting water from entering the environment.
Protection during firefighting	: Do not enter fire area without proper protective equipment, including respiratory protection.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures	: Remove ignition sources. Prevent from entering sewers, basements and workpits, or any place where its accumulation can be dangerous. Avoid contact with skin and eyes.
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6.1.1. For non-emergency personnel

Emergency procedures	: Evacuate unnecessary personnel.
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6.1.2. For emergency responders

Protective equipment	: Equip cleanup crew with proper protection. Use personal protective equipment as required. Dust/aerosol mask. Safety glasses. Protective gloves.
Emergency procedures	: Ventilate area.

6.2. Environmental precautions

Prevent entry to sewers and public waters. Notify authorities if liquid enters sewers or public waters.

6.3. Methods and material for containment and cleaning up

Methods for cleaning up	: On land, sweep or shovel into suitable containers. Minimise generation of dust. Store away from other materials.
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6.4. Reference to other sections

See Section 8. Exposure controls and personal protection.

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SECTION 7: Handling and storage

7.1. Precautions for safe handling

- Precautions for safe handling : Avoid dust formation. Do not breathe dust. Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Do not handle until all safety precautions have been read and understood. Use only outdoors or in a well-ventilated area.
- Hygiene measures : Wash hands, forearms and face thoroughly after handling.

7.2. Conditions for safe storage, including any incompatibilities

- Storage conditions : Store at room temperature. Keep only in the original container in a cool, well ventilated place away from : Oxidizing agent, Heat sources, Direct sunlight. Keep container tightly closed.
- Incompatible products : Strong bases. Strong acids.
- Incompatible materials : Sources of ignition. Direct sunlight.

7.3. Specific end use(s)

Active Ingredient for Medicinal/Pharmaceutical Use.

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 : MOEHS occupational exposure band: 2 (0.1 - 1 mg/m³)

8.2. Exposure controls

8.2.1. Appropriate engineering controls

No additional information available

8.2.2. Personal protection equipment

Personal protective equipment:

Avoid all unnecessary exposure. Gloves. Safety glasses. Dust/aerosol mask with filter type P3.

Personal protective equipment symbol(s):



8.2.2.1. Eye and face protection

Eye protection:

Chemical goggles or safety glasses

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Eye protection		
Type	Field of application	Standard
Safety glasses	Dust, Fine dust	EN 166

8.2.2.2. Skin protection

Skin and body protection:

Wear suitable protective clothing

Skin and body protection	
Type	Standard
Disposable gowns, Reusable gowns, Tyvek® Gown/Coveralls	EN 13034, EN 1149-1

Hand protection:

Wear protective gloves.

Hand protection		
Type	Material	Standard
Disposable gloves	Nitrile rubber (NBR), Butyl rubber, Natural rubber, Latex, Vinyl, Polyvinylchloride (PVC), Neoprene rubber (HNBR), Fluoroelastomer (FKM)	EN 374-2

Other skin protection

Materials for protective clothing

Condition	Material	Standard
Good resistance:	Synthetic material, Tyvek®, Polyethylene	EN 13034, EN ISO 13982-1

8.2.2.3. Respiratory protection

Respiratory protection:

Wear appropriate mask

Respiratory protection			
Device	Filter type	Condition	Standard
Dust mask	Type P3	High dust protection	EN 143

8.2.2.4. Thermal hazards

No additional information available

8.2.3. Environmental exposure controls

Other information:

Do not eat, drink or smoke during use.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Solid
Colour	: white to slightly yellow.
Molecular mass	: 461.82 g/mol
Odour	: characteristic.
Odour threshold	: Not available
Melting point	: 116 – 118 °C [Sitagliptin base]

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Freezing point	: Not available
Boiling point	: 469.9 – 589.9 °C [at 760 mmHg; ACD/LABS Sitagliptin base]
Flammability	: Non flammable.
Explosive limits	: Not applicable
Lower explosion limit	: Not applicable
Upper explosion limit	: Not applicable
Flash point	: 241.4 – 307.2 °C [ACD/LABS Sitagliptin base]
Auto-ignition temperature	: Not applicable
Decomposition temperature	: Not available
pH	: Not available
pH solution	: Not available
Viscosity, kinematic	: Not applicable
Solubility	: Not available
Partition coefficient n-octanol/water (Log Kow)	: Not available
Vapour pressure	: Not available
Vapour pressure at 50°C	: Not available
Density	: Not available
Relative density	: Not available
Relative vapour density at 20°C	: Not applicable
Particle size	: Not available
Particle size distribution	: Not available
Particle shape	: Not available
Particle aspect ratio	: Not available
Particle aggregation state	: Not available
Particle agglomeration state	: Not available
Particle specific surface area	: Not available
Particle dustiness	: Not available

9.2. Other information

9.2.1. Information with regard to physical hazard classes

No additional information available

9.2.2. Other safety characteristics

Additional information : Minimum ignition energy : 200-300 mJ (Electrostatic).
Dust Cloud minimum Flammability Temperature : 510°C.
Layer Minimum flammability Temperature : >400°C.
Explosivity Pmax : 8.6 Bar.
Explosion Severity Factor Kmax (bar.m/s) : 187.
Explosion Class : St1

SECTION 10: Stability and reactivity

10.1. Reactivity

No additional information available

10.2. Chemical stability

Not established.

10.3. Possibility of hazardous reactions

Not established.

10.4. Conditions to avoid

Direct sunlight. Extremely high or low temperatures.

10.5. Incompatible materials

Strong acids. Strong bases.

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10.6. Hazardous decomposition products

fume. Carbon monoxide. Carbon dioxide.

SECTION 11: Toxicological information

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Acute toxicity (oral) : Not classified
Acute toxicity (dermal) : Not classified
Acute toxicity (inhalation) : Not classified

SITAGLIPTIN HYDROCHLORIDE MONOHYDRATE (862156-92-1)

LD50 oral rat	> 2000 mg/kg
Skin corrosion/irritation	: Causes skin irritation.
Serious eye damage/irritation	: Causes serious eye irritation.
Respiratory or skin sensitisation	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Germ cell mutagenicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Carcinogenicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Reproductive toxicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
STOT-single exposure	: May cause respiratory irritation.
STOT-repeated exposure	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Aspiration hazard	: Not classified
Additional information	: Based on available data, the classification criteria are not met

11.2. Information on other hazards

11.2.1. Endocrine disrupting properties

Adverse health effects caused by endocrine disrupting properties : The substance is not included in the list established in accordance with Article 59(1) of REACH for having endocrine disrupting properties, or is not identified as having endocrine disrupting properties in accordance with the criteria set out in Commission Delegated Regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605

11.2.2. Other information

Potential adverse human health effects and symptoms : Based on available data, the classification criteria are not met

SECTION 12: Ecological information

12.1. Toxicity

Hazardous to the aquatic environment, short-term (acute) : Not classified
Hazardous to the aquatic environment, long-term (chronic) : Not classified

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LC50 - Fish [1]	> 100 mg/l [Minnow]
EC50 - Crustacea [1]	60 mg/l
EC50 96h - Algae [1]	31 mg/l

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12.2. Persistence and degradability

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Persistence and degradability	Not readily biodegradable.
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12.3. Bioaccumulative potential

SITAGLIPTIN HYDROCHLORIDE MONOHYDRATE (862156-92-1)

BCF - Fish [1]	2.347 [Predicted by BCFWIN v2.17]
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Bioaccumulative potential	Not established.
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12.4. Mobility in soil

SITAGLIPTIN HYDROCHLORIDE MONOHYDRATE (862156-92-1)

Organic Carbon Normalized Adsorption Coefficient (Log Koc)	6.383 [Predicted by PCKOCWIN v1.66]
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12.5. Results of PBT and vPvB assessment

No additional information available

12.6. Endocrine disrupting properties

Adverse effects on the environment caused by endocrine disrupting properties : The substance/mixture has no endocrine disrupting properties.

12.7. Other adverse effects

Additional information : Avoid release to the environment.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Product/Packaging disposal recommendations : Dispose in a safe manner in accordance with local/national regulations.
Ecology - waste materials : Avoid release to the environment.

SECTION 14: Transport information

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

14.1. UN number or ID number

UN-No. (ADR) : Not applicable
UN-No. (IMDG) : Not applicable
UN-No. (IATA) : Not applicable
UN-No. (ADN) : Not applicable
UN-No. (RID) : Not applicable

14.2. UN proper shipping name

Proper Shipping Name (ADR) : Not applicable
Proper Shipping Name (IMDG) : Not applicable
Proper Shipping Name (IATA) : Not applicable
Proper Shipping Name (ADN) : Not applicable
Proper Shipping Name (RID) : Not applicable

14.3. Transport hazard class(es)

ADR
Transport hazard class(es) (ADR) : Not applicable

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IMDG

Transport hazard class(es) (IMDG) : Not applicable

IATA

Transport hazard class(es) (IATA) : Not applicable

ADN

Transport hazard class(es) (ADN) : Not applicable

RID

Transport hazard class(es) (RID) : Not applicable

14.4. Packing group

Packing group (ADR) : Not applicable
Packing group (IMDG) : Not applicable
Packing group (IATA) : Not applicable
Packing group (ADN) : Not applicable
Packing group (RID) : Not applicable

14.5. Environmental hazards

Dangerous for the environment : No
Marine pollutant : No
Other information : 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. Maritime transport in bulk according to IMO instruments

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

REACH Annex XVII (Restriction List)

Not listed on REACH Annex XVII

REACH Annex XIV (Authorisation List)

Not listed on REACH Annex XIV (Authorisation List)

REACH Candidate List (SVHC)

Not listed on the REACH Candidate List

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PIC Regulation (Prior Informed Consent)

Not listed on the PIC list (Regulation EU 649/2012)

POP Regulation (Persistent Organic Pollutants)

Not listed on the POP list (Regulation EU 2019/1021)

Ozone Regulation (1005/2009)

Not listed on the Ozone Depletion list (Regulation EU 1005/2009)

Explosives Precursors Regulation (2019/1148)

Contains no substance(s) listed on the Explosives Precursors list (Regulation EU 2019/1148 on the marketing and use of explosives precursors)

Drug Precursors Regulation (273/2004)

Contains no substance(s) listed on the Drug Precursors list (Regulation EC 273/2004 on the manufacture and the placing on market of certain substances used in the illicit manufacture of narcotic drugs and psychotropic substances)

15.1.2. National regulations

Germany

Water hazard class (WGK) : Not classified according to Regulation Governing Systems for Handling Substances Hazardous to Waters (AwSV).
Hazardous Incident Ordinance (12. BImSchV) : Is not subject of the Hazardous Incident Ordinance (12. BImSchV)

Netherlands

SZW-lijst van kankerverwekkende stoffen : The substance is not listed
SZW-lijst van mutagene stoffen : The substance is not listed
SZW-lijst van reprotoxische stoffen – Borstvoeding : The substance is not listed
SZW-lijst van reprotoxische stoffen – Vruchtbaarheid : The substance is not listed
SZW-lijst van reprotoxische stoffen – Ontwikkeling : The substance is not listed

Denmark

Danish National Regulations : Young people below the age of 18 years are not allowed to use the product

Switzerland

Storage class (LK) : LK 11/13 - Solids

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
BCF	Bioconcentration factor
CLP	Classification Labelling Packaging Regulation; Regulation (EC) No 1272/2008
DMEL	Derived Minimal Effect level
DPD	Dangerous Preparations Directive 1999/45/EC
DSD	Dangerous Substances Directive 67/548/EEC
EC50	Median effective concentration
IATA	International Air Transport Association
IMDG	International Maritime Dangerous Goods
LD50	Median lethal dose
LC50	Median lethal concentration

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Abbreviations and acronyms:

LOAEL	Lowest Observed Adverse Effect Level
vPvB	Very Persistent and Very Bioaccumulative

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.

Other information : None.

Full text of H- and EUH-statements:

Eye Irrit. 2	Serious eye damage/eye irritation, Category 2
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
Skin Irrit. 2	Skin corrosion/irritation, Category 2
STOT SE 3	Specific target organ toxicity – Single exposure, Category 3, Respiratory tract irritation

Safety Data Sheet (SDS), EU

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.