

SAFETY DATA SHEET

according to 1907/2006/EC, Article 3

Version no. : 2.1
Prepared on : 22.12.2022
Revised on : 18.11.2025

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

1.1 Product identifiers

Product name 4-(6- Fluorobenzo[d]isoxazol3-yl)-1-[2-(9-hydroxy-2- methyl-4-oxo-6,7,8,9-tetrahydro-4Hpyrido[1,2-a]pyrimidin-3- yl)ethyl]piperidine-1- oxide
Product Number PSR40741
Brand PureSynth research chemicals
CAS No. 761460-08-6

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

Identified uses : Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company PureSynth Research Chemicals GmbH
64683 Einhausen Marie-Curie-StraBe. 3, Germany

1.4 Emergency telephone number

Worldwide Helpline No.: 1800-8908-260

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008

Acute toxicity, (Category 3) H301: Toxic if swallowed.

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram



Signal word

Danger

Hazard statement(s)

H301 Toxic if swallowed.

Precautionary statement(s)

P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P405 Store locked up.
P501 Dispose of contents/ container to an approved waste disposal plant.
Supplemental Hazard Statements none

2.3 Other hazards:

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or

very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Ecological information: The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Toxicological information: The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher

SECTION 3: Composition / information on ingredients

3.1 Substances

Common names & Synonyms	Mol. formula	CAS number
Paliperidone N-oxide 3-[2-[4-(6-fluoro-1,2-benzoxazol-3-yl)-1-oxido-piperidin-1-ium1-yl]ethyl]-9-hydroxy-2-methyl-6,7,8,9-tetrahydropyrido[1,2- a]pyrimid	C ₂₃ H ₂₇ FN ₄ O ₄	761460-08-6
Component	Classification	Concentration
Flourobenzel{d}isoxale	Acute Tox. 3; H301	<= 100 %

SECTION 4: First aid measures

Description of first aid measures

General advice	Show this safety data sheet to the doctor in attendance.
If inhaled	After inhalation: fresh air.
In case of skin contact	In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.
In case of eye contact	After eye contact: rinse out with plenty of water. Remove contact lenses.
If swallowed	If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.
Most important symptoms and effects, both acute and delayed	The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11
Indication of any immediate medical attention and special treatment needed	No data available

SECTION 5: Firefighting measures

Extinguishing media	
Suitable extinguishing media	No data available
Unsuitable extinguishing media	For this substance/mixture no limitations of extinguishing agents are given.
Special hazards arising from the substance or mixture	Carbon oxides Nitrogen oxides (NOx) Hydrogen fluoride
Advice for fire-fighters	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	Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water

system.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures	Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.
Environmental precautions	Do not let product enter drains.
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 carefully. Dispose of properly. Clean up affected area. Avoid generation of dusts.
Reference to other sections	For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling	For precautions see section 2.2.
Conditions for safe storage, including any incompatibilities	Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorised persons. Storage stability: Recommended storage temperature 2 - 8 °C Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects
Specific end use(s)	Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls / Personal protection

Control parameters	Ingredients with workplace control parameters
Exposure controls	
Appropriate engineering controls	No data available
Personal protective equipment:	
Eye / face protection	Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses
Skin protection	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 EN 16523-1 please contact the supplier of CE-approved gloves Full contact Material: Nitrile rubber Minimum layer thickness: 0.11 mm Break through time: 480 min Splash contact Material: Nitrile rubber Minimum layer thickness: 0.11 mm Break through time: 480 min
Body Protection	protective clothing
Respiratory protection	required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: Filter type P3

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.

Do not let product enter drains.

Control of environmental exposure

SECTION 9: Physical and chemical properties

Appearance	Form: Solid
	Colour: White
Odour	No data available
pH - Value	No data available
Density	No data available
Boiling Point	No data available
Melting Point	160 - 162 °C - Decomposition
Solubility in water	No data available
Flash point	Not applicable
Vapour pressure	No data available
Auto -ignition temperature	No data available
Vapour density	No data available
Flammability (solid, gas)	No data available
Evaporation rate	No data available
Partition coefficient: n- octanol / water	No data available
Viscosity	No data available
Explosive properties	Not classified as explosive.
Upper / lower flammability or explosive limits	No data available
Oxidizing properties	none
Other safety information:	
Solubility in other solvents	Methanol - slightly soluble

SECTION 10: Stability and reactivity

Reactivity	No data available
Chemical stability	The product is chemically stable under standard ambient conditions (room temperature).
Possibility of hazardous reactions	No data available
Condition to avoid	no information available
Incompatible materials	Strong oxidizing agents
Hazardous decomposition products	In the event of fire: see section 5

SECTION 11: Toxicological information

Acute toxicity	Oral: No data available Inhalation: No data available
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	Dermal: No data available
Skin corrosion/irritation	No data available
Serious eye damage/eye irritation	No data available
Respiratory or skin sensitization	No data available
Germ cell mutagenicity	No data available
Carcinogenicity	No data available
Reproductive toxicity	No data available
Specific target organ toxicity - single exposure	No data available
Specific target organ toxicity - repeated exposure	No data available
Aspiration hazard	No data available
Additional Information	<p>The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.</p> <p>To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.</p>

SECTION 12: Ecological information.

Toxicity

Toxicity to fish	No data available
Toxicity to daphnia and other aquatic invertebrates	No data available
Toxicity to algae	No data available
Toxicity to bacteria	No data available
Toxicity to fish(Chronic toxicity)	No data available
Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)	No data available
Persistence and degradability	No data available
Bioaccumulation	No data available
Mobility in soil	No data available

Results of PBT and vPvB assessment This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Endocrine disrupting properties The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Other adverse effects No data available

SECTION 13: Disposal considerations

Waste treatment methods	No data available
Contaminated packaging	No data available.

SECTION 14: Transport information

	UN no.	UN proper shipping name	Hazard Class(es)	Packaging group	Marine Pollutant
ADR / RID	2811	TOXIC SOLID, ORGANIC, N.O.S. (3-[2-[4-(6-fluoro-1,2-benzoxazol-3-yl)-1-oxido-piperidin-1-ium-1-yl]ethyl]-9-hydroxy-2-methyl-6,7,8,9-tetrahydropyrido[1,2-a]pyrimidin-4-one)	6.1	III	no
IMDG	2811	TOXIC SOLID, ORGANIC, N.O.S. (3-[2-[4-(6-fluoro-1,2-benzoxazol-3-yl)-1-oxido-piperidin-1-ium-1-yl]ethyl]-9-hydroxy-2-methyl-6,7,8,9-tetrahydropyrido[1,2-a]pyrimidin-4-one)	6.1	III	no
IATA	2811	Toxic solid, organic, n.o.s. (3-[2-[4-(6-fluoro-1,2-benzoxazol-3-yl)-1-oxidopiperidin-1-ium-1-yl]ethyl]-9-hydroxy-2-methyl-6,7,8,9-tetrahydropyrido[1,2-a]pyrimidin-4-one)	6.1	III	no

SECTION 15: Regulatory information

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

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

National legislation

H2 ACUTE TOXIC

Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances.

15.2 Chemical safety assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

The information in this SDS is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. The user must be determined suitability of this information for his application.