

**Safety Data Sheet**

according to UK REACH Regulation

**Fmoc-L-His-Aib-OH\*TFA**

Revision date: 05.07.2024

Product code: FDP1440

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

Fmoc-L-His-Aib-OH\*TFA

**Further trade names**

N-alpha-(9-Fluorenylmethyloxycarbonyl)-L-histidyl-aminoisobutyric acid trifluoroacetate

Fmoc-His-Aib-OH trifluoroacetate

(S)-2-(2-(((9H-fluoren-9-yl)methoxy)carbonyl)amino)-3-(1H-imidazol-4-yl)propanamido)-2-methylpropanoic acid trifluoroacetate salt

2-[[[(2S)-2-(9H-fluoren-9-ylmethoxycarbonylamino)-3-(1H-imidazol-5-yl)propanoyl]amino]-2-methyl-propanoic acid trifluoroacetic acid salt

Substance name: Fmoc-L-His-Aib-OH\*TFA  
REACH Registration Number: 01-2120880119-49-XXXX  
CAS No: 1446013-08-6  
EC No: 815-122-7

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

Laboratory chemical. Manufacture of the substance.

**Uses advised against**

Do not use for private purposes (household).

Restrictions on use: Pharmaceutical substance

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

Company name: Iris Biotech GmbH  
Street: Adalbert-Zoellner-Straße 1  
Place: D-95615 Marktredwitz, Germany  
Post-office box: 568  
D-95605 Marktredwitz, Germany  
Telephone: +49 9231 97121 0  
Telefax: +49 9231 97121 99  
E-mail: info@iris-biotech.de  
Contact person: Health & Safety Department  
Telephone: +49 9231 97121 0  
E-mail: sds@iris-biotech.de  
Internet: www.iris-biotech.de  
Responsible Department: Only available during office hours.

**1.4. Emergency telephone number:** +49 (0)89 19240 (POISON CENTER Munich: 24 h)**SECTION 2: Hazards identification****2.1. Classification of the substance or mixture****GB CLP Regulation**

Eye Dam. 1; H318

Full text of hazard statements: see SECTION 16.

**2.2. Label elements****GB CLP Regulation****Signal word:** Danger

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**Pictograms:**

**Hazard statements**

H318 Causes serious eye damage.

**Precautionary statements**

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

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

P310 Immediately call a POISON CENTER/doctor.

**Additional advice on labelling**

Warning - substance not yet tested completely.

**2.3. Other hazards**

Product is not dust explosive in its original delivery form. The addition of particulate matter, however, results in a dust explosion risk.

**SECTION 3: Composition/information on ingredients**
**3.1. Substances**
**Chemical characterization**

N-alpha-(9-Fluorenylmethyloxycarbonyl)-L-histidyl-aminoisobutyric acid trifluoroacetate

 Sum formula: C<sub>25</sub>H<sub>26</sub>N<sub>4</sub>O<sub>5</sub>\*CF<sub>3</sub>CO<sub>2</sub>H

Molecular weight: 462,51\*114,02 g/mol

**Relevant ingredients**

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (GB CLP Regulation)			
1446013-08-6	Fmoc-L-His-Aib-OH*TFA			100 %
	815-122-7		01-2120880119-49-XXXX	
	Eye Dam. 1; H318			

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

**Specific Conc. Limits, M-factors and ATE**

CAS No	EC No	Chemical name	Quantity
	Specific Conc. Limits, M-factors and ATE		
1446013-08-6	815-122-7	Fmoc-L-His-Aib-OH*TFA	100 %
	oral: LD50 = ca. 5000 mg/kg		

**SECTION 4: First aid measures**
**4.1. Description of first aid measures**
**General information**

In case of accident or unwellness, seek medical advice immediately (show directions for use or safety data sheet if possible).

In all cases of doubt, or when symptoms persist, seek medical advice.

**After inhalation**

Provide fresh air. Remove casualty to fresh air and keep warm and at rest. In case of irregular breathing or respiratory arrest provide artificial respiration.

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**After contact with skin**

Wash with plenty of water. Take off contaminated clothing and wash it before reuse. After contact with skin, wash immediately with plenty of water and soap.

**After contact with eyes**

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist.

**After ingestion**

Rinse mouth thoroughly with water. Never give anything by mouth to an unconscious person or a person with cramps.

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

No information available.

**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**

Co-ordinate fire-fighting measures to the fire surroundings. Water spray. alcohol resistant foam. Dry extinguishing powder. Sand.

**Unsuitable extinguishing media**

High power water jet.

**5.2. Special hazards arising from the substance or mixture**

Non-flammable. Thermal decomposition can lead to the escape of irritating gases and vapours.

In case of fire may be liberated: Carbon dioxide (CO<sub>2</sub>). Carbon monoxide (CO). Nitrogen oxides (NO<sub>x</sub>).

Hydrogen fluoride (HF).

**5.3. Advice for firefighters**

In case of fire: Wear self-contained breathing apparatus.

**Additional information**

Suppress gases/vapours/mists with water spray jet. Collect contaminated fire extinguishing water separately.

Do not allow entering drains or surface water. Usual measures for fire prevention.

**SECTION 6: Accidental release measures****6.1. Personal precautions, protective equipment and emergency procedures****General advice**

Provide adequate ventilation. Avoid dust formation. Do not breathe dust. Avoid contact with skin, eyes and clothes. Use personal protection equipment. Provide adequate ventilation. Avoid breathing dust/fume/gas/mist/vapours/spray.

Avoid contact with skin, eyes and clothes.

Wear personal protection equipment.

In case of fire: Evacuate area.

**For non-emergency personnel**

Remove all sources of ignition. Provide adequate ventilation.

Use personal protection equipment.

**For emergency responders**

Wear personal protection equipment (refer to section 8).

Take up mechanically, placing in appropriate containers for disposal. Take up dust-free and set down dust-free.

**6.2. Environmental precautions**

Do not allow to enter into soil/subsoil.

Do not allow to enter into surface water or drains.

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**6.3. Methods and material for containment and cleaning up****For containment**

Avoid dust formation.

**For cleaning up**

Take up mechanically. Treat the recovered material as prescribed in the section on waste disposal. Take up mechanically.

**Other information**Take up mechanically, placing in appropriate containers for disposal. Avoid dust formation.  
Clear contaminated areas thoroughly.**6.4. Reference to other sections**

Safe handling: see section 7

Personal protection equipment: see section 8

Disposal: see section 13

Treat the recovered material as prescribed in the section on waste disposal.

**SECTION 7: Handling and storage****7.1. Precautions for safe handling****Advice on safe handling**If handled uncovered, arrangements with local exhaust ventilation have to be used. Avoid dust formation. Do not breathe dust. Provide adequate ventilation.  
Avoid breathing dust/fume/gas/mist/vapours/spray.  
Avoid contact with skin, eyes and clothes.**Advice on protection against fire and explosion**

Usual measures for fire prevention.

**Advice on general occupational hygiene**Remove contaminated, saturated clothing immediately. Draw up and observe skin protection programme.  
Wash hands and face before breaks and after work and take a shower if necessary. When using do not eat, drink, smoke, sniff. Take off contaminated clothing. Wash hands before breaks and after work. When using do not eat, drink, smoke, sniff. Avoid contact with skin, eyes and clothes. Provide adequate ventilation.**7.2. Conditions for safe storage, including any incompatibilities****Requirements for storage rooms and vessels**Keep container tightly closed. Keep container tightly closed in a cool, well-ventilated place.  
Handle and store contents under inert gas. Protect from moisture.  
storage temperature: room temperature**Hints on joint storage**

No special measures are necessary.

**7.3. 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****8.1. Control parameters****Additional advice on limit values**

To date, no national critical limit values exist.

**8.2. Exposure controls**

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**Appropriate engineering controls**

If handled uncovered, arrangements with local exhaust ventilation have to be used. Do not breathe dust. The receiver of our product is singularly responsible for adhering to existing laws and regulations.

**Individual protection measures, such as personal protective equipment****Eye/face protection**

Suitable eye protection: goggles.

Tightly fitting safety goggles. Face shield (8-inch minimum). Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

**Hand protection**

When handling with chemical substances, protective gloves must be worn with the CE-label including the four control digits. The quality of the protective gloves resistant to chemicals must be chosen as a function of the specific working place concentration and quantity of hazardous substances. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. Wear suitable gloves.

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands. The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

**Skin protection**

Use of protective clothing.

**Respiratory protection**

In case of inadequate ventilation wear respiratory protection. If technical exhaust or ventilation measures are not possible or insufficient, respiratory protection must be worn.

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

**Thermal hazards**

No data available

**Environmental exposure controls**

Discharge into the environment must be avoided.

**SECTION 9: Physical and chemical properties****9.1. Information on basic physical and chemical properties**

Physical state:	solid	
Colour:	white/ whitish	
Odour:	No data available	
Odour threshold:	No data available	
Melting point/freezing point:		No data available
Boiling point or initial boiling point and boiling range:		No data available
Flammability:		not determined
Lower explosion limits:		No data available

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Upper explosion limits:	No data available
Flash point:	No data available
Auto-ignition temperature:	No data available
Decomposition temperature:	No data available
pH-Value:	No data available
Viscosity / kinematic:	not applicable
Water solubility: (at 23 °C)	0.001 g/L
Solubility in other solvents not determined	
Dissolution rate:	No data available
Partition coefficient n-octanol/water:	No data available
Dispersion stability:	No data available
Vapour pressure: (at 20 °C)	0,0017 hPa
Vapour pressure: (at 50 °C)	0,0017 hPa
Density:	0,54 g/cm <sup>3</sup>
Relative density:	No data available
Bulk density:	No data available
Relative vapour density:	No data available
Particle characteristics:	No data available

**9.2. Other information****Information with regard to physical hazard classes**

## Explosive properties

The product is not: Explosive. Product is not dust explosive in its original delivery form. The addition of particulate matter, however, results in a dust explosion risk.

Sustaining combustion: No data available

## Self-ignition temperature

Solid:

No data available

Gas:

not applicable

## Oxidizing properties

No data available

**Other safety characteristics**

Solvent content:

No data available

Viscosity / dynamic:

not applicable

Flow time:

not applicable

**SECTION 10: Stability and reactivity****10.1. Reactivity**

No data available

**10.2. Chemical stability**

Stable under recommended storage conditions.

**10.3. Possibility of hazardous reactions**

No data available

**10.4. Conditions to avoid**

Protect from moisture.

Keep away from heat.

**10.5. Incompatible materials**

Oxidizing agents, strong.

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**10.6. Hazardous decomposition products**

Thermal decomposition can lead to the escape of irritating gases and vapours.

In case of fire may be liberated: Carbon dioxide (CO<sub>2</sub>). Carbon monoxide (CO). Nitrogen oxides (NO<sub>x</sub>).

Hydrogen fluoride (HF).

**Further information**

In case of fire: See chapter 5.

**SECTION 11: Toxicological information****11.1. Information on hazard classes as defined in GB CLP Regulation****Toxicokinetics, metabolism and distribution**

No data available

**Acute toxicity**

Based on available data, the classification criteria are not met.

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
1446013-08-6	Fmoc-L-His-Aib-OH*TFA				
	oral	LD50 mg/kg	ca. 5000	Rat	Study report (2019) OECD Guideline 423

**Irritation and corrosivity**

Serious eye damage/eye irritation: Causes serious eye damage.

Skin corrosion/irritation: Based on available data, the classification criteria are not met.

**Sensitising effects**

Based on available data, the classification criteria are not met.

**Carcinogenic/mutagenic/toxic effects for reproduction**

Germ cell mutagenicity: Based on available data, the classification criteria are not met.

Carcinogenicity: Based on available data, the classification criteria are not met.

Reproductive toxicity: Based on available data, the classification criteria are not met.

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

**STOT-single exposure**

Based on available data, the classification criteria are not met.

**STOT-repeated exposure**

Based on available data, the classification criteria are not met.

**Aspiration hazard**

Based on available data, the classification criteria are not met.

**Information on likely routes of exposure**

No data available

**Specific effects in experiment on an animal**

No data available

**Practical experience**

No data available

**11.2. Information on other hazards****Endocrine disrupting properties**

No data available

**Other information**

This substance is classified as hazardous according to Regulation (EC) No 1272 (2008).

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Fluoride ion can reduce serum calcium levels possibly causing fatal hypocalcemia.

**Further information**

RTECS: No data available

To our knowledge, the chemical, physical and toxicological properties have not been extensively studied. Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

**SECTION 12: Ecological information**
**12.1. Toxicity**

Based on available data, the classification criteria are not met.

CAS No	Chemical name					
	Aquatic toxicity	Dose	[h]   [d]	Species	Source	Method
1446013-08-6	Fmoc-L-His-Aib-OH*TFA					
	Acute algae toxicity	ErC50 > 50,8 mg/l	72 h	Desmodesmus subspicatus	Study report (2021)	OECD Guideline 201
	Acute crustacea toxicity	EC50 > 322,2 mg/l	48 h	Daphnia magna	Study report (2021)	OECD Guideline 202

**12.2. Persistence and degradability**

No data available

**12.3. Bioaccumulative potential**

No data available

**Partition coefficient n-octanol/water**

CAS No	Chemical name	Log Pow
1446013-08-6	Fmoc-L-His-Aib-OH*TFA	0,651

**12.4. Mobility in soil**

No data available

**12.5. Results of PBT and vPvB assessment**

This substance does not meet the PBT/vPvB criteria of UK REACH.

The product has not been tested.

**12.6. Endocrine disrupting properties**

This substance does not have endocrine disrupting properties with respect to non-target organisms.

**12.7. Other adverse effects**

Warning - substance not yet tested completely.

**Further information**

Do not allow to enter into surface water or drains. Do not allow to enter into soil/subsoil.

Avoid release to the environment.

**SECTION 13: Disposal considerations**
**13.1. Waste treatment methods**
**Disposal recommendations**

Do not allow to enter into surface water or drains. Do not allow to enter into soil/subsoil. Dispose of waste according to applicable legislation.

Consult the appropriate local waste disposal expert about waste disposal.

Handle contaminated packages in the same way as the substance itself.

**Contaminated packaging**

Non-contaminated packages may be recycled. Handle contaminated packages in the same way as the substance itself.



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**SECTION 14: Transport information****Land transport (ADR/RID)****14.2. UN proper shipping name:** No dangerous good in sense of these transport regulations.**Inland waterways transport (ADN)****14.2. UN proper shipping name:** No dangerous good in sense of these transport regulations.**Marine transport (IMDG)****14.2. UN proper shipping name:** No dangerous good in sense of these transport regulations.**Air transport (ICAO-TI/IATA-DGR)****14.2. UN proper shipping name:** No dangerous good in sense of these transport regulations.**14.5. Environmental hazards**

ENVIRONMENTALLY HAZARDOUS: No

**14.6. Special precautions for user**

No information available.

**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****EU regulatory information**

Information according to Directive 2012/18/EU (SEVESO III): Not subject to 2012/18/EU (SEVESO III)

**Additional information**

Safety Data Sheet according to Regulation (EC) No. 1907/2006 (REACH)

**National regulatory information**

Employment restrictions: Observe restrictions to employment for juveniles according to the 'juvenile work protection guideline' (94/33/EC).

Water hazard class (D): 3 - highly hazardous to water

**15.2. Chemical safety assessment**

For this substance a chemical safety assessment has not been carried out.

**SECTION 16: Other information**

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**Abbreviations and acronyms**

Eye Dam: Eye damage

ADR: Accord relatif au transport international des marchandises dangereuses par route  
(Agreement concerning the International Carriage of Dangerous Goods by Road).

IMDG: International Maritime Code for Dangerous Goods

IATA: International Air Transport Association

GHS: Globally Harmonized System of Classification and Labelling of Chemicals

EINECS: European Inventory of Existing Commercial Chemical Substances

ELINCS: European List of Notified Chemical Substances

CAS: Chemical Abstracts Service

LC50: Lethal concentration, 50%

LD50: Lethal dose, 50%

CLP: Classification, labelling and Packaging

REACH: Registration, Evaluation and Authorization of Chemicals

GHS: Globally Harmonised System of Classification, Labelling and Packaging of Chemicals

UN: United Nations

CAS: Chemical Abstracts Service

DNEL: Derived No Effect Level

DMEL: Derived Minimal Effect Level

PNEC: Predicted No Effect Concentration

ATE: Acute toxicity estimate

LL50: Lethal loading, 50%

EL50: Effect loading, 50%

EC50: Effective Concentration 50%

ErC50: Effective Concentration 50%, growth rate

NOEC: No Observed Effect Concentration

BCF: Bio-concentration factor

PBT: persistent, bioaccumulative, toxic

vPvB: very persistent, very bioaccumulative

RID: Regulations concerning the international carriage of dangerous goods by rail

ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways  
(Accord européen relatif au transport international des marchandises dangereuses par voies de navigation  
intérieures)

EmS: Emergency Schedules

MFAG: Medical First Aid Guide

IATA: International Air Transport Association

ICAO: International Civil Aviation Organization

MARPOL: International Convention for the Prevention of Marine Pollution from Ships

IBC: Intermediate Bulk Container

SVHC: Substance of Very High Concern

For abbreviations and acronyms, see table at <http://abbrev.esdscom.eu>

EC/EEC: European Community/European Economic Community

EU: European Union

M-factor: Multiplying factor

ADR: Accord européen sur le transport des marchandises dangereuses par Route

(European Agreement concerning the International Carriage of Dangerous Goods by Road)

IATA: International Air Transport Association

DGR: Dangerous Goods Regulations

ICAO: International Civil Aviation Organization

TI: Technical Instructions

For abbreviations and acronyms, see: ECHA Guidance on information requirements and chemical safety  
assessment, chapter R.20 (Table of terms and abbreviations).**Relevant H and EUH statements (number and full text)**

H318 Causes serious eye damage.

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#### Further Information

The information is based on the present level of our knowledge. It does not, however, give assurance of product properties and establishes no contract legal rights. The receiver of our product is singularly responsible for adhering to existing laws and regulations.