

Safety Data Sheet

according to UK REACH Regulation

ATFB

Revision date: 09.08.2018

Product code: RL-2035

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

ATFB

Further trade names

4-Azido-2,3,5,6-tetrafluorobenzoic acid

4-Azido-2,3,5,6-tetrafluoro-benzoic acid

N3-TFBA

3-(4-carboxy-2,3,5,6-tetrafluorophenyl)-2?5-triaz-1-en-2-yn-3-ium-1-ide

CAS No: 122590-77-6

EC No: 802-636-1

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

Use as laboratory reagent.

Scientific research and development.

Uses advised against

Do not use for private purposes (household).

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
e-mail: info@iris-biotech.de
Contact person: Compliance Department
e-mail: sds@iris-biotech.de
Internet: www.iris-biotech.de
Responsible Department: Only available during office hours.

Telefax: +49 9231 97121 99

Telephone: +49 9231 97121 0

1.4. Emergency telephone

+49 (0)89 19240 (POISON CENTER Munich: 24 h)

number:**Further Information**

Emergency telephone: 24 h

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

Hazard categories:

Flammable solid: Flam. Sol. 2

Skin corrosion/irritation: Skin Irrit. 2

Serious eye damage/eye irritation: Eye Irrit. 2

Specific target organ toxicity - single exposure: STOT SE 3

Hazard Statements:

Flammable solid.

Causes skin irritation.

Causes serious eye irritation.

May cause respiratory irritation.

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

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Pictograms:

Hazard statements

H228	Flammable solid.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.

Precautionary statements

P261	Avoid breathing dust/fume/gas/mist/vapours/spray.
P264	Wash hands thoroughly after handling.
P280	Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
P302+P352	IF ON SKIN: Wash with plenty of water.
P332+P313	If skin irritation occurs: Get medical advice/attention.
P362+P364	Take off contaminated clothing and wash it before reuse.
P304+P340	IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P312	Call a POISON CENTER/doctor if you feel unwell.
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337+P313	If eye irritation persists: Get medical advice/attention.
P403+P233	Store in a well-ventilated place. Keep container tightly closed.
P405	Store locked up.
P501	Dispose of contents/container to an approved disposal site.

Additional advice on labelling

Warning - substance not yet tested completely.

2.3. Other hazards

No data available

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

4-Azido-2,3,5,6-tetrafluorobenzoic acid

Sum formula: C7HF4N3O2

Molecular weight: 235,10 g/mol

Hazardous components

CAS No	Chemical name	Quantity
	EC No	
	Index No	
	REACH No	
	GHS Classification	
122590-77-6	4-Azido-2,3,5,6-tetrafluorobenzoic acid	<= 100 %
	802-636-1	
	Flam. Sol. 2, Skin Irrit. 2, Eye Irrit. 2, STOT SE 3; H228 H315 H319 H335	

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

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Specific Conc. Limits, M-factors and ATE

CAS No	EC No	Chemical name	Quantity
		Specific Conc. Limits, M-factors and ATE	
122590-77-6	802-636-1	4-Azido-2,3,5,6-tetrafluorobenzoic acid	<= 100 % %
		inhalation: Data lacking (gases); dermal: Data lacking; oral: Data lacking	

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).

After inhalation

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

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

After contact with skin

After contact with skin, wash immediately with polyethylene glycol, followed by plenty of water. Take off immediately all contaminated clothing and wash it before reuse. If skin irritation occurs: Get medical advice/attention. After contact with skin, wash immediately with plenty of water and soap.

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

After contact with eyes

After contact with the eyes, rinse with water with the eyelids open for a sufficient length of time, then consult an ophthalmologist immediately. In case of contact with eyes, rinse immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart. Subsequently consult an ophthalmologist.

After ingestion

Rinse mouth immediately and drink plenty of water. Rinse mouth thoroughly with water. Never give anything by mouth to an unconscious person or a person with cramps.

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

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

No data available

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

Treat symptomatically. 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. Carbon dioxide (CO₂). Sand.

Unsuitable extinguishing media

High power water jet.

5.2. Special hazards arising from the substance or mixture

Flammable. Vapours can form explosive mixtures with air. Thermal decomposition can lead to the escape of irritating gases and vapours.

In case of fire may be liberated: Carbon dioxide (CO₂). Carbon monoxide (CO). Nitrogen oxides (NO_x).

Fluorhydric acid.

5.3. Advice for firefighters

Wear a self-contained breathing apparatus and chemical protective clothing. Full protection suit.

Additional information

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

Do not allow entering drains or surface water.

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Usual measures for fire prevention.

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

Remove all sources of ignition. 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.

Wear personal protection equipment.

In case of fire: Evacuate area.

6.2. Environmental precautions

Do not allow uncontrolled discharge of product into the environment. Danger of explosion Do not allow to enter into soil/subsoil.

Do not allow to enter into surface water or drains.

6.3. Methods and material for containment and cleaning up**Other information**

Take up mechanically. Treat the recovered material as prescribed in the section on waste disposal. 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 dust formation. Avoid breathing dust/fume/gas/mist/vapours/spray.

Avoid contact with skin, eyes and clothes.

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

Use explosion-proof electrical equipment.

Advice on protection against fire and explosion

Keep away from sources of ignition - No smoking. Take precautionary measures against static discharges.

Vapours can form explosive mixtures with air. 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 or drink. Avoid contact with skin, eyes and clothes. Provide adequate ventilation. When using do not eat, drink or smoke. Wash hands before breaks and after work.

Further information on handling

Handle with care - avoid bumps, friction and impact.

7.2. Conditions for safe storage, including any incompatibilities**Requirements for storage rooms and vessels**

Keep container tightly closed. Keep in a cool, well-ventilated place. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Keep container tightly closed in a cool, well-ventilated place.

Handle and store contents under inert gas. Protect from moisture.

storage temperature: -20 °C

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Hints on joint storage

Do not store together with: Oxidizing agent. Pyrophoric or self-heating substances.

Further information on storage conditions

Sensitive to air

Sensitivity to light.

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**

No data available

8.2. Exposure controls**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. Wear eye/face protection.

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.

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.

Skin protection

Wear suitable protective clothing. Wear suitable 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.

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:	whitish/ light yellow
Odour:	No data available

Changes in the physical state

Melting point/freezing point: 139 - 141 °C

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Boiling point or initial boiling point and boiling range:	No data available
Sublimation point:	No data available
Softening point:	No data available
Flash point:	No data available
Flammability	
Solid/liquid:	No data available
Gas:	not applicable
Explosive properties	
No data available	
Lower explosion limits:	No data available
Upper explosion limits:	No data available
Auto-ignition temperature:	No data available
Self-ignition temperature	
Solid:	not determined
Gas:	not applicable
Decomposition temperature:	not determined
Oxidizing properties	
No data available	
pH-Value:	No data available
Water solubility:	No data available
Solubility in other solvents	
Soluble in: Chloroform (CHCl ₃). Methanol (CH ₃ OH). Dimethylsulfoxide (DMSO).	
Partition coefficient n-octanol/water:	No data available
Vapour pressure:	No data available
Density:	No data available
Bulk density:	No data available
Relative vapour density:	not determined

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

Sustaining combustion: No data available

Other safety characteristics

Solvent content: No data available

Solid content: not determined

Evaporation rate: not determined

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

Flammable.

10.2. Chemical stability

Stable under recommended storage conditions.

10.3. Possibility of hazardous reactions

Risk of explosion by shock, friction, fire or other sources of ignition.

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10.4. Conditions to avoid

Protect from moisture.
Keep away from heat.
Protect from sunlight. Photosensitive.

10.5. Incompatible materials

Oxidizing agents, strong.
acid.

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 (CO₂). Carbon monoxide (CO). Nitrogen oxides (NO_x).
Fluorhydric acid.

Contact with acids liberates toxic gas.

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
122590-77-6	4-Azido-2,3,5,6-tetrafluorobenzoic acid				
	oral	Data lacking			
	dermal	Data lacking			
	inhalation	Data lacking			

Irritation and corrosivity

Causes skin irritation.
Causes serious eye irritation.

Sensitising effects

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

Carcinogenic/mutagenic/toxic effects for reproduction

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

May cause respiratory irritation. (4-Azido-2,3,5,6-tetrafluorobenzoic acid)

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.

Specific effects in experiment on an animal

No data available

Additional information on tests

Classification according to Regulation (EC) No 1272/2008 [CLP]: health hazard properties

Practical experience

No data available

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Further information

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

100 percent of the mixture consists of ingredient(s) of unknown toxicity.

Warning - substance not yet tested completely.

SECTION 12: Ecological information
12.1. Toxicity

No data available

CAS No	Chemical name					
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method
122590-77-6	4-Azido-2,3,5,6-tetrafluorobenzoic acid					
	Aquatic toxicity	Data lacking				

12.2. Persistence and degradability

No data available

12.3. Bioaccumulative potential

No data available

12.4. Mobility in soil

No data available

12.5. Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

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.

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

Dispose of waste according to applicable legislation. Dispose of waste according to applicable legislation.

Consult the appropriate local waste disposal expert about waste disposal.

Contaminated packaging

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

SECTION 14: Transport information
Land transport (ADR/RID)
14.1. UN number:

UN 1325

14.2. UN proper shipping name:

 FLAMMABLE SOLID, ORGANIC, N.O.S.
 (4-Azido-2,3,5,6-tetrafluorobenzoic acid)

14.3. Transport hazard class(es):

4.1

14.4. Packing group:

III

Hazard label:

4.1



Classification code:

F1

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Special Provisions: 274
 Limited quantity: 5 kg
 Excepted quantity: E1
 Transport category: 3
 Hazard No: 40
 Tunnel restriction code: E

Inland waterways transport (ADN)

14.1. UN number: UN 1325
14.2. UN proper shipping name: FLAMMABLE SOLID, ORGANIC, N.O.S.
 (4-Azido-2,3,5,6-tetrafluorobenzoic acid)
14.3. Transport hazard class(es): 4.1
14.4. Packing group: III
 Hazard label: 4.1



Classification code: F1
 Special Provisions: 274
 Limited quantity: 5 kg
 Excepted quantity: E1

Marine transport (IMDG)

14.1. UN number: UN 1325
14.2. UN proper shipping name: FLAMMABLE SOLID, ORGANIC, N.O.S.
 (4-Azido-2,3,5,6-tetrafluorobenzoic acid)
14.3. Transport hazard class(es): 4.1
14.4. Packing group: III
 Hazard label: 4.1



Special Provisions: 223, 274, 915
 Limited quantity: 5 kg
 Excepted quantity: E1
 EmS: F-A, S-G

Air transport (ICAO-TI/IATA-DGR)

14.1. UN number: UN 1325
14.2. UN proper shipping name: FLAMMABLE SOLID, ORGANIC, N.O.S.
 (4-Azido-2,3,5,6-tetrafluorobenzoic acid)
14.3. Transport hazard class(es): 4.1
14.4. Packing group: III
 Hazard label: 4.1



Special Provisions: A3 A803
 Limited quantity Passenger: 10 kg
 Passenger LQ: Y443
 Excepted quantity: E1
 IATA-packing instructions - Passenger: 446

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IATA-max. quantity - Passenger:	25 kg
IATA-packing instructions - Cargo:	449
IATA-max. quantity - Cargo:	100 kg

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: No

14.6. Special precautions for user

Warning: flammable solids.

14.7. Maritime transport in bulk according to IMO instruments

not applicable

Other applicable information

No data available

SECTION 15: Regulatory information**15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture****EU regulatory information**

Information according to 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**Abbreviations and acronyms**

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

Relevant H and EUH statements (number and full text)

H228	Flammable solid.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.

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. Warning - substance not yet tested completely.

The product is intended for research, analysis and scientific education.

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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 above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.