

Safety Data Sheet

SFP-Piperazinyipyridine

according to Regulation (EU) nr. 1907/2006

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

Product name SFP-Piperazinyipyridine

Product code RO4909902-000

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

Use - intermediate in the synthesis of an active pharmaceutical compound

1.3. Details of the supplier of the safety data sheet

Company information

Enquiries:
F. Hoffmann-La Roche AG
Postfach
CH-4070 Basel
Switzerland

Local representation:

Phone +41-61/688 54 80
Fax +41-61/681 72 76
E-Mail info.sds@roche.com

1.4. Emergency telephone number

Emergency telephone number Phone +41-61/688 54 80

SFP-Piperazinylpyridine

SECTION 2: Hazards identification

2.1. / 2.2. Classification of the substance or mixture / Label elements

GHS Classification

Health Hazards:

- 3.1 Acute toxicity (Category 3)
H301 Toxic if swallowed.
- 3.2 Skin corrosion/irritation (Category 1B)
H314 Causes severe skin burns and eye damage.

Environmental Hazards:

- 4.1 Hazardous to the aquatic environment (Category 2)
H411 Toxic to aquatic life with long lasting effects.

Signalword: Danger

Label:



Precautionary statements:

- P273 Avoid release to the environment.
- P280 Wear protective gloves/ protective clothing / eye protection / face protection.
- P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
- P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
- P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
- P309 + P310 IF exposed or if you feel unwell: Immediately call a POISON CENTER or doctor/physician.

2.3. Other hazards

Note

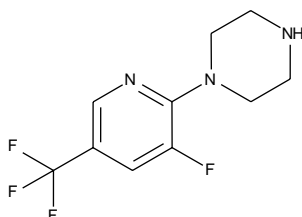
- may form explosible dust-air mixture if dispersed

SECTION 3: Composition/information on ingredients

Chemical name	- 1-(3-Fluoro-5-trifluoromethyl-pyridin-2-yl)-piperazine
CAS number	845616-81-1
UN number	2923
Roche number	RO4909902-000
Empirical formula	C ₁₀ H ₁₁ F ₄ N ₃

SFP-Piperazinyipyridine

Molecular mass 249.21 g/mol



SECTION 4: First aid measures

4.1. Description of first aid measures

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|--------------|--|
| Eye contact | <ul style="list-style-type: none">- rinse immediately with tap water for 10 minutes - open eyelids forcibly- consult a physician |
| Skin contact | <ul style="list-style-type: none">- remove contaminated clothing immediately and drench affected skin with plenty of water |
| Inhalation | <ul style="list-style-type: none">- get medical treatment immediately- avoid mouth to mouth artificial respiration, use respiration equipment |

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

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| Note | <ul style="list-style-type: none">- no information available |
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4.3. Indication of any immediate medical attention and special treatment needed

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|-------------------|--|
| Note to physician | <ul style="list-style-type: none">- treat symptomatically- in case of strong exposure betamimetics and topical and/or systemic steroids as needed; subsequent follow-up because of possible latency of pulmonary symptoms |
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SECTION 5: Firefighting measures

5.1. Extinguishing media

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|------------------------------|---|
| Suitable extinguishing media | <ul style="list-style-type: none">- water spray jet, dry powder, foam, carbon dioxide |
|------------------------------|---|

5.2. Special hazards arising from the substance or mixture

- | | |
|------------------|---|
| Specific hazards | <ul style="list-style-type: none">- heating of container(s) will cause pressure rise with risk of bursting and subsequent explosion- may attack metals and produce hydrogen gas which may form explosive mixture with air- gives off toxic and corrosive fumes, also when burning |
|------------------|---|

5.3. Advice for firefighters

Protection of fire-fighters	<ul style="list-style-type: none">- precipitate gases/vapours/mists with water spray- chemical incident emergency response unit with full protective equipment
Special method of fire-fighting	<ul style="list-style-type: none">- cool endangered containers with water spray- for reasons of environmental protection hold the extinguishing agent back

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Personal precautions	<ul style="list-style-type: none">- if this is not endangering the action force or other people, ventilate sewers and cellars
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6.2. Environmental precautions

Environmental protection	<ul style="list-style-type: none">- if possible close leaks- collect the leaked product by all means available- if the substance reaches waters or the sewer system, inform the competent authority
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6.3. Methods and material for containment and cleaning up

Methods for cleaning up	<ul style="list-style-type: none">- collect solids (avoid dust formation) and hand over to waste removal- collect liquids by means of sand, earth or another suitable material- use acid resistant equipment- collect the product spilled out into ventilated containers equipped with absorption filters
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SECTION 7: Handling and storage

7.1. Precautions for safe handling

Technical measures	<ul style="list-style-type: none">- avoid dust formation; very high dust explosion hazard- processing in closed systems, if possible superposed by inert gas (e.g. nitrogen)- take precautionary measures against electrostatic charging- local exhaust ventilation necessary
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7.2. Conditions for safe storage, including any incompatibilities

Storage conditions	<ul style="list-style-type: none">- protected from heat, light and humidity
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SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Threshold value (Roche) air - Category D (Roche Group Directive K1, Annex 3): OEL = 10 µg/m³

8.2. Exposure controls

General protective and hygiene measures - instruction of employees recommended

Respiratory protection - in case of open handling or accidental release:
particle mask or respirator with independent air supply

Hand protection - protective gloves (eg made of neoprene, nitrile or butyl rubber)

Eye protection - safety glasses

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Colour white

Form solid

Solubility soluble, toluene
4'750 mg/l, water (20 °C, OECD No. 105)

Partition coefficient log P_{ow} 1.29 (octanol/water) pH 7.0
(HPLC Method, OECD No. 117)

Melting temperature 61.5 °C (OECD No. 102)

9.2. Other information

Note - no information available

SECTION 10: Stability and reactivity

10.1. Reactivity

Note - no information available

10.2. Chemical stability

Note - no information available

10.3. Possibility of hazardous reactions

Note - no information available

10.4. Conditions to avoid

Conditions to avoid - temperatures above 50 °C

10.5. Incompatible materials

Note - no information available

10.6. Hazardous decomposition products

Note - autocatalytic, very violent exothermal decomposition with an extremely high decomposition rate

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity - LD₅₀ ~ 200 mg/kg (oral, rat)
(OECD No. 423 (Acute Toxic Class Method))

Local effects - skin: corrosive (rabbit; OECD No. 404)

Mutagenicity - negative, both with and without metabolic activation (Ames test; OECD No. 471 (Salmonella typhimurium, Escherichia coli))

SECTION 12: Ecological information

12.1. Toxicity

Ecotoxicity - strongly toxic for algae (Desmodesmus (=Scenedesmus) subspicatus)
ErC₅₀ (72 h) 2.73 mg/l
NOErC (72 h) 0.97 mg/l
EyC₅₀ (72 h) 1.21 mg/l
NOEyC (72 h) 0.55 mg/l
(OECD No. 201)

- inhibition of substrate degradation in the biodegradability test (activated sludge)
concentration (28 d) 51.5 mg/l (measured initial concentration)
(Manometric Respirometry Test, OECD No. 301 F)

12.2. Persistence and degradability

Ready biodegradability - not readily biodegradable
0 % BOD/ThOD, 28 d
(Manometric Respirometry Test, OECD No. 301 F)

Inherent biodegradability - not inherently biodegradable
0 %, 28 d
(flask shaking test Roche Basel, inherent biodegradation)

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Abiotic degradation - hydrolytically stable at environmentally relevant pH values

12.3. Bioaccumulative potential

Note - no information available

12.4. Mobility in soil

Note - no information available

12.5. Results of PBT and vPvB assessment

PBT/vPvB - substance does not meet the criteria for PBT or vPvB

12.6. Other adverse effects

Note - no information available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Waste from residues - observe local/national regulations regarding waste disposal

SECTION 14: Transport information

IATA	Class	UN/ID	PG		PI	Label	Mark
	8 & 6.1	2923	III		860/864	8 & 6.1	EHS

IMDG	Class	UN	PG	EmS	PI	Label	Mark
	8 & 6.1	2923	III	F-A S-B	P002/IBC08	8 & 6.1	marine pollutant

RID/ADR	Class	UN	PG	Haz.no	PI	Label	Mark	Classif. code
	8 & 6.1	2923	III	86	P002/IBC08	8 & 6.1	EHS	CT2

Proper shipping name CORROSIVE SOLID, TOXIC, N.O.S.

Technical name 1-(3-Fluoro-5-trifluoromethyl-pyridin-2-yl)-piperazine

SECTION 15: Regulatory information

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

Water hazard class (Germany)	3: strongly hazardous for water (own classification according to directive VwVwS of 27.07.2005)
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SECTION 16: Other information

Safety-lab number	- BS-8692 - BS-8646
Edition documentation	- changes from previous version in sections 2, 8

The information in this safety data sheet is based on current scientific knowledge. It should not be taken as expressing or implying any warranty concerning product characteristics.