

## Safety Data Sheet

according to Regulation (EC) No 1907/2006 (REACH)  
Classifications according to Regulation (EC) No 1272/2008.  
Printdate 24 Sep 2024

## 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

### 1.1. Product name:

Bicyclopyrone Metabolite SYN 545910

### 1.1. Catalog No.:

686362

### 1.2. Relevant identified uses of the substance or mixture

Identified: Laboratory chemical  
uses: R&D

### 1.3. Uses advised against:

HPC Standards GmbH  
Am Wieseneck 7

04451 Cunnersdorf  
Deutschland

Tel. +49 34291 3372-36  
Fax. +49 34291 3372-39  
contact@hpc-standards.com

### 1.4. Emergency telephone number

HPC Standards Tel. +49 34291 3372-36  
This number is only available during office hours.

## 2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

Flammable liquids (Category 2), H225

Acute toxicity, Oral (Category 4), H302

Acute toxicity, Inhalation (Category 4), H332

Acute toxicity, Dermal (Category 4), H312

Eye irritation (Category 2), H319

For the full text of the H-Statements mentioned in this Section, see Section 16.

F Highly flammable R11

Xn Harmful R20/21/22

Xi Irritant R36

### 2.2. Label elements

#### 2.2.1. Pictogram



### 2.2.2.

Signal word Danger

Hazard statement(s)

Highly flammable liquid and vapour. Harmful if swallowed, in contact with skin or if inhaled. Causes serious eye irritation. Wear protective gloves and protective clothing. Wear eye or face protection. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Avoid breathing vapour. Do not eat, drink or smoke when using this product. IF INHALED: Call a POISON CENTER or doctor if you feel unwell. Dispose of contents and container in accordance with all local, regional, national and international regulations.

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms : Methyl cyanide

ACN

Formula : C<sub>2</sub>H<sub>3</sub>N

Molecular weight : 41,05 g/mol

CAS-No. : 75-05-8

EC-No. : 200-835-2

Index-No. : 608-001-00-3

Component:

Acetonitrile

CAS-No. 75-05-8

EC-No. 200-835-2

Index-No. 608-001-00-3

Classification:

Flam. Liq. 2; Acute Tox. 4; Eye Irrit. 2; H225, H302, H332, H312, H319

Concentration:

<= 100 %

### 3.1.1. Formula

C<sub>10</sub>H<sub>10</sub>F<sub>3</sub>NO<sub>4</sub>

### 3.1.2. Molecular Weight (g/mol)

265.19

### 3.1.3. CAS-No.

## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

#### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

#### In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

#### If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

### 4.2 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

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

no data available

## 5. FIRE-FIGHTING MEASURES

### 5.1 Extinguishing media

#### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

### 5.2 Special hazards arising from the substance or mixture

no data available

### 5.3 Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

### 5.4 Further information

Use water spray to cool unopened containers.

## 6. ACCIDENTAL RELEASE MEASURES

### 6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation.

Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

For personal protection see section 8.

### 6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

### 6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

### 6.4 Reference to other sections

For disposal see section 13.

## 7. HANDLING AND STORAGE

### 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

### 7.2 Conditions for safe storage, including any incompatibilities

Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Recommended storage temperature: 2 - 8 °C

### 7.3 Specific end uses

no data available

## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

Components with workplace control parameters

Derived No Effect Level (DNEL)

Application Area Workers

Exposure routes Inhalation

Health effect Acute local effects, Acute systemic effects

Value 68 mg/m<sup>3</sup>

Application Area Workers

Exposure routes Skin contact

Health effect Long-term systemic effects

Value 32,2mg/kg BW/d

Application Area Workers

Exposure routes Inhalation

Health effect Long-term local effects, Long-term systemic effects

Value 68 mg/m<sup>3</sup>

Application Area Workers

Exposure routes Inhalation

Health effect Long-term local effects, Long-term systemic effects

Value 68 mg/m<sup>3</sup>

Application Area Consumers

Exposure routes Inhalation

Health effect Acute local effects

Value 220 mg/m<sup>3</sup>

Application Area Consumers

Exposure routes Inhalation

Health effect Acute systemic effects

Value 22 mg/m<sup>3</sup>

Application Area Consumers

Exposure routes Inhalation

Health effect Long-term systemic effects

Value 4,8 mg/m<sup>3</sup>

### Predicted No Effect Concentration (PNEC)

Compartment	Value
Water	10 mg/l
Soil	2,41 mg/kg
Marine water	1 mg/l
Fresh water	10 mg/l
Fresh water sediment	7,53 mg/kg
Onsite sewage treatment plant	32 mg/l

### 8.2 Exposure controls

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching gloves 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.

If used in solution, or mixed with other substances, and under conditions which

differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

#### Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing.. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

#### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a fullface 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).

#### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

a) Appearance Form: clear, liquid

Colour: colourless

b) Odour ether-like

c) Odour Threshold no data available

d) pH no data available

e) Melting point/freezing point

Melting point/range: -48 °C

f) Initial boiling point and boiling range

81 - 82 °C

g) Flash point 2,0 °C - closed cup

h) Evaporation rate 5,8

i) Flammability (solid, gas) no data available

j) Upper/lower flammability or

explosive limits

Upper explosion limit: 16 %(V)

Lower explosion limit: 3 %(V)

k) Vapour pressure 73,18 hPa at 15 °C

121,44 hPa at 25 °C

413,23 hPa at 55 °C

98,64 hPa at 20 °C

l) Vapour density 1,42 - (Air = 1.0)

m) Relative density 0,786 g/mL at 25 °C

n) Water solubility completely soluble

o) Partition coefficient: noctanol/

water

log Pow: -0,54 at 25 °C

p) Auto-ignition

temperature

524,0 °C

q) Decomposition

temperature

no data available

r) Viscosity no data available

s) Explosive properties Not explosive

t) Oxidizing properties The substance or mixture is not classified as oxidizing.

### 9.2 Other safety information

Surface tension 29,0 mN/m at 20,0 °C

Relative vapour density 1,42 - (Air = 1.0)

## 10. STABILITY AND REACTIVITY

- 10.1 Reactivity  
no data available
- 10.2 Chemical stability  
no data available
- 10.3 Possibility of hazardous reactions  
no data available
- 10.4 Conditions to avoid  
Heat, flames and sparks. Extremes of temperature and direct sunlight.
- 10.5 Incompatible materials  
acids, Bases, Oxidizing agents, Alkali metals
- 10.6 Hazardous decomposition products  
Other decomposition products - no data available

## 11. TOXICOLOGICAL INFORMATION

- 11.1 Information on toxicological effects
  - Acute toxicity
  - LD50 Oral - rat - male - 1.320 - 6.690 mg/kg
  - LC50 Inhalation - mouse - 4 h - 3587 ppm  
(OECD Test Guideline 403)
  - LC50 Inhalation - rat - 4 h - 26,8 mg/l
  - LD50 Dermal - rabbit - male and female - > 2.000 mg/kg  
(OECD Test Guideline 402)
  - Skin corrosion/irritation
  - Skin - rabbit
  - Result: No skin irritation  
(OECD Test Guideline 404)
  - Serious eye damage/eye irritation
  - Eyes - rabbit
  - Result: Irritating to eyes.  
(OECD Test Guideline 405)
  - Respiratory or skin sensitisation
  - Buehler Test - guinea pig
  - Did not cause sensitisation on laboratory animals.  
(OECD Test Guideline 406)
  - Germ cell mutagenicity
  - Hamster
  - ovary
  - Result: negative
  - Mutation in mammalian somatic cells.
  - Ames test
  - S. typhimurium
  - Result: Not mutagenic in Ames Test.
  - Hamster
  - ovary
  - Result: Equivocal evidence.
  - Sister chromatid exchange
  - Mutagenicity (micronucleus test)
  - mouse
  - Result: Positive results were obtained in some in vivo tests.
  - Carcinogenicity
  - No evidence of carcinogenicity in animal studies (when indicated)
  - 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.
  - Reproductive toxicity
  - Animal testing did not show any effects on fertility.
  - Specific target organ toxicity - single exposure
  - The substance or mixture is not classified as specific target organ toxicant, single exposure.
  - Specific target organ toxicity - repeated exposure
  - The substance or mixture is not classified as specific target organ toxicant, repeated exposure.
  - Aspiration hazard
  - No aspiration toxicity classification
  - Additional Information
  - RTECS: AL7700000
  - Treat as cyanide poisoning., Always have on hand a cyanide first-aid kit, together with proper instructions., The onset of symptoms is generally delayed pending conversion to cyanide., Nausea, Vomiting, Diarrhoea, Headache, Dizziness, Rash, Cyanosis, excitement, depression, Drowsiness, impaired judgment, Lack of coordination, stupor, death

## 12. ECOLOGICAL INFORMATION

- 12.1 Toxicity  
no data available
- 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  
no data available
- 12.6 Other adverse effects  
no data available

## 13. DISPOSAL CONSIDERATIONS

- 13.1 Waste treatment methods  
Product  
Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company.
- Contaminated packaging  
Dispose of as unused product.

## 14. TRANSPORT INFORMATION

- 14.1 UN number  
ADR/RID: 1648 IMDG: 1648 IATA: 1648
- 14.2 UN proper shipping name  
ADR/RID: ACETONITRILE  
IMDG: ACETONITRILE  
IATA: Acetonitrile
- 14.3 Transport hazard class(es)  
ADR/RID: 3 IMDG: 3 IATA: 3
- 14.4 Packaging group  
ADR/RID: II IMDG: II IATA: II
- 14.5 Environmental hazards  
ADR/RID: no IMDG Marine Pollutant: no IATA: no
- 14.6 Special precautions for user  
no data available

## 15. REGULATORY INFORMATION

- This safety datasheet complies with the requirements of the regulation named on the first page of this SDS.
- 15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture  
no data available
- 15.2 Chemical Safety Assessment  
no data available

## 16. OTHER INFORMATION

The above information 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. It does not represent any guarantee of the properties of the product. For lab use only!