

Chemical Safety Data Sheet MSDS / SDS

1H-Pyrazole-4-carboxaldehyde, 1-(2,2-difluoroethyl)-3,5-dimethyl-

Revision Date:2026-08-29 Revision Number:1

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

Product name : 1H-Pyrazole-4-carboxaldehyde, 1-(2,2-difluoroethyl)-3,5-dimethyl-
CBnumber : CB010439281
CAS : 1006487-12-2
Synonyms : 1-(2,2-Difluoroethyl)-3,5-dimethyl-1H-pyrazole-4-carbaldehyde

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 010-86108875

SECTION 2: Hazards identification**GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Warning

Precautionary statements

P391 Collect spillage. Hazardous to the aquatic environment
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P273 Avoid release to the environment.
P264 Wash skin thoroughly after handling.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

Hazard statements

H410 Very toxic to aquatic life with long lasting effects
H319 Causes serious eye irritation
H317 May cause an allergic skin reaction
H315 Causes skin irritation

SECTION 3: Composition/information on ingredients

Substance

Product name	: 1H-Pyrazole-4-carboxaldehyde, 1-(2,2-difluoroethyl)-3,5-dimethyl-
Synonyms	: 1-(2,2-Difluoroethyl)-3,5-dimethyl-1H-pyrazole-4-carbaldehyde
CAS	: 1006487-12-2
MF	: C ₈ H ₁₀ F ₂ N ₂ O
MW	: 188.17

SECTION 4: 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

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2) and/or in section 11

Protection of first-aiders

For personal protection see section 8.

Notes to physician

No data available

SECTION 5: Firefighting measures

Suitable extinguishing media

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

Hazardous combustion products

Carbon oxides Nitrogen oxides (NOx) Hydrogen fluoride

Specific extinguishing methods

No data available

Special protective equipment for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Avoid breathing dust. Advice for emergency responders: For personal protection see section 8.

Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

SECTION 7: Handling and storage

Handling

Advice on protection against fire and explosion

Provide appropriate exhaust ventilation at places where dust is formed.

Advice on safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.

Avoidance of contact

Strong oxidizing agents

Storage

Conditions for safe storage

Keep container tightly closed in a dry and wellventilated place.

Storage class

11, Combustible Solids

Recommended storage temperature

Recommended storage temperature see product label.

SECTION 8: Exposure controls/personal protection

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures

No data available

Personal protective equipment

Respiratory protection

For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges.

Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

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 EN 166(EU).

Skin and body protection

Complete suit protecting against chemicals

The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Hand protection

Remarks

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.

Hygiene measures

Handle in accordance with good industrial hygiene and safety practice.

Wash hands before breaks and at the end of workday.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

solid

Color

No data available

Odor

No data available

Odor Threshold

No data available

pH

No data available

Melting point/ range

No data available

Boiling point/boiling range

267.6±40.0 °C(Predicted)

Flash point

Not applicable

Evaporation rate

No data available

Flammability (solid, gas)

No data available

Flammability (liquids)

No data available

Burning rate

No data available

Upper explosion limit / Upper flammability limit

No data available

Lower explosion limit / Lower flammability limit

No data available

Vapor pressure

No data available

Relative vapor density

No data available

Relative density

1.25±0.1 g/cm³(Predicted)

Density

1.25±0.1 g/cm³(Predicted)

Water solubility

slightly soluble (25 °C)

Partition coefficient: n-octanol/water

log Pow: -0.69 (25 °C)

Method: (calculated) Bioaccumulation is not expected.

Autoignition temperature

No data available

Decomposition temperature

No data available

Viscosity, dynamic

No data available

Viscosity, kinematic

No data available

Flow time

No data available

Explosive properties

No data available

Oxidizing properties

none

Molecular weight

188.18 g/mol

Particle characteristics Particle size

No data available

Physical state

solid

SECTION 10: Stability and reactivity**Reactivity**

No data available

Chemical stability

No data available

Possibility of hazardous reactions

Stable under recommended storage conditions.

Conditions to avoid

No data available

Incompatible materials

Strong oxidizing agents

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Acute toxicity estimate Oral - 1,080 mg/kg (Expert judgement)

Remarks: The value / statement given is based on a (Q)SAR approach

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

Remarks: The value / statement given is based on a (Q)SAR approach

Serious eye damage/eye irritation

Remarks: The value / statement given is based on a (Q)SAR approach

Respiratory or skin sensitization

The value / statement given is based on a (Q)SAR approach

Germ cell mutagenicity

Classified based on available data. For more details, see section 2

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

Classified based on available data. For more details, see section 2

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

Ecotoxicity

Components:

1-(2,2-difluoroethyl)-3,5-dimethyl-1H-pyrazole-4-carbaldehyde:

Ecotoxicology Assessment

Chronic aquatic toxicity

Very toxic to aquatic life with long lasting effects. Remarks: The value / statement given is based on a (Q)SAR approach

Persistence and degradability

Components:

1-(2,2-difluoroethyl)-3,5-dimethyl-1H-pyrazole-4-carbaldehyde:

Biodegradability

Result: Not readily biodegradable. Remarks: The value / statement given is based on a (Q)SAR approach

Bioaccumulative potential

Components:

1-(2,2-difluoroethyl)-3,5-dimethyl-1H-pyrazole-4-carbaldehyde:

Partition coefficient: octanol/water

log Pow: -0.69 (25 °C) Method: (calculated) Remarks: Bioaccumulation is not expected.

Mobility in soil

No data available

Other adverse effects

Additional ecological information

Very toxic to aquatic life with long lasting effects.

SECTION 13: Disposal considerations

Disposal methods

Waste from residues

Offer surplus and non-recyclable solutions to a licensed disposal company. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

International Regulations

IATA-DGR

UN/ID No. : UN 3077

Proper shipping name : Environmentally hazardous substance, solid, n.o.s.

(1-(2,2-difluoroethyl)-3,5-dimethyl-1H-pyrazole-4carbaldehyde)

Class : 9

Packing group : III

Labels : Class 9 - Miscellaneous dangerous substances and articles

Packing instruction (cargo aircraft) : 956

Packing instruction (passenger aircraft) : 956

IMDG-Code

UN number : UN 3077

Proper shipping name : ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.

(1-(2,2-difluoroethyl)-3,5-dimethyl-1H-pyrazole-4carbaldehyde)

Class : 9

Packing group : III

Labels : 9

EmS Code : F-A, S-F

Marine pollutant : yes

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable for product as supplied.

National Regulations

JT/T 617

UN number : UN 3077

Proper shipping name : ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.

(1-(2,2-difluoroethyl)-3,5-dimethyl-1H-pyrazole-4carbaldehyde)

Class : 9

Packing group : III

Labels : 9

Environmentally hazardous : no

Special precautions for user

Remarks : EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous

Goods > 5L for liquids or > 5kg for solids.

Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15: Regulatory information

Catalogue of Hazardous Chemicals : This product is not listed in the catalogue of hazardous chemicals, but it meets the definition of hazardous chemicals and its principles of determination.

Downstream users need to comply with the conditions of safe use of the chemical, understand the environmental and health hazard and risk management measures identified on the SDS as well as the local/national regulations concerning the chemical.

National regulatory information

Regulations on Safety Management of Hazardous Chemicals

Identification of Major Hazard Installations for Hazardous Chemicals (GB 18218)

Not listed

Hazardous Chemicals for Priority Management

Not listed under SAWS

Regulations on Labour Protection in Workplaces where Toxic Substances are Used

Catalogue of Highly Toxic Chemicals

Not listed

Regulation of Environmental Management on the First Import of Chemicals and the Import and Export of Toxic Chemicals

China Severely Restricted Toxic Chemicals for Import and Export

Not listed

Measures on the Environmental Administration of New Chemical Substances Registration

Registration/Notification number

B1A222241205

SECTION 16: Other information

Full text of other abbreviations

AIIIC - Australian Inventory of Industrial Chemicals

ANTT - National Agency for Transport by Land of Brazil

ASTM - American Society for the Testing of Materials

bw - Body weight

CMR - Carcinogen, Mutagen or Reproductive Toxicant

DIN - Standard of the German Institute for Standardisation

DSL - Domestic Substances List (Canada)

EC_x - Concentration associated with x% response

EL_x - Loading rate associated with x% response

EmS - Emergency Schedule

ENCs - Existing and New Chemical Substances (Japan)

ErC_x - Concentration associated with x% growth rate response

ERG - Emergency Response Guide
 GHS - Globally Harmonised System
 GLP - Good Laboratory Practice
 IARC - International Agency for Research on Cancer
 IATA - International Air Transport Association
 IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk
 IC50 - Half maximal inhibitory concentration
 ICAO - International Civil Aviation Organization
 IECSC - Inventory of Existing Chemical Substances in China
 IMDG - International Maritime Dangerous Goods
 IMO - International Maritime Organisation
 ISHL - Industrial Safety and Health Law (Japan)
 ISO - International Organisation for Standardisation
 KECI - Korea Existing Chemicals Inventory
 LC50 - Lethal Concentration to 50 % of a test population
 LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose)
 MARPOL - International Convention for the Prevention of Pollution from Ships
 MERCOSUR - The Agreement for the Facilitation of the Transport of Dangerous Goods
 n.o.s. - Not Otherwise Specified
 Nch - Chilean Norm
 NO(A)EC - No Observed (Adverse) Effect Concentration
 NO(A)EL - No Observed (Adverse) Effect Level
 NOELR - No Observable Effect Loading Rate
 NOM - Official Mexican Norm
 NTP - National Toxicology Program
 NZIoC - New Zealand Inventory of Chemicals
 OECD - Organisation for Economic Co-operation and Development
 OPPTS - Office of Chemical Safety and Pollution Prevention
 PBT - Persistent, Bioaccumulative and Toxic substance
 PICCS - Philippines Inventory of Chemicals and Chemical Substances
 (Q)SAR - (Quantitative) Structure Activity Relationship
 REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals
 SADT - Self-Accelerating Decomposition Temperature
 SDS - Safety Data Sheet
 TCSI - Taiwan Chemical Substance Inventory
 TDG - Transportation of Dangerous Goods
 TECI - Thailand Existing Chemicals Inventory
 TSCA - Toxic Substances Control Act (United States)
 UN - United Nations
 UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods
 vPvB - Very Persistent and Very Bioaccumulative
 WHMIS - Workplace Hazardous Materials Information System

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.