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Safety Data Sheet

according to Regulation (EC) No 1907/2006 (REACH)
Classifications according to Regulation (EC) No 1272/2008.
Printdate 16 Dec 2025

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

1.1. Product name:

Pyflubumide-des(2-methyl-1-oxopropyl)

1.1. Catalog No.:

690605

1.2. Relevant identified uses of the substance or mixture

Identified: Laboratory chemical
uses: R&D

1.3. Uses advised against:

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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

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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 : C2H3N
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

C21H25F6N3O2

3.1.2. Molecular Weight (g/mol)

465.43

3.1.3. CAS-No.

926914-68-3

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/m3
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/m3
Application Area Workers
Exposure routes Inhalation
Health effect Long-term local effects, Long-term systemic effects
Value 68 mg/m3
Application Area Consumers
Exposure routes Inhalation
Health effect Acute local effects
Value 220 mg/m3
Application Area Consumers
Exposure routes Inhalation
Health effect Acute systemic effects
Value 22 mg/m3
Application Area Consumers
Exposure routes Inhalation
Health effect Long-term systemic effects
Value 4,8 mg/m3

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) Evapouration 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

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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!