1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifier

Product name: KHK-IN-1 (hydrochloride)
Catalog No.: HY-12841A
CAS No.: 1303470-48-5

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

Identified uses: Laboratory chemicals, manufacture of substances.

1.3 Details of the supplier of the safety data sheet

Company: MedChemExpress USA
Tel: 609-228-6898
Fax: 609-228-5909
E-mail: sales@medchemexpress.com

1.4 Emergency telephone number

Emergency Phone #: 609-228-6898

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

Not a hazardous substance or mixture.

2.2 GHS Label elements, including precautionary statements

Not a hazardous substance or mixture.

2.3 Other hazards

None.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms: ketohexokinase inhibitor
Formula: C_{12}H_{17}ClIN_{5}S
Molecular Weight: 459.01
CAS No.: 1303470-48-5

4. FIRST AID MEASURES

4.1 Description of first aid measures

Eye contact
Remove any contact lenses, locate eye-wash station, and flush eyes immediately with large amounts of water. Separate eyelids with fingers to ensure adequate flushing. Promptly call a physician.

Skin contact
Rinse skin thoroughly with large amounts of water. Remove contaminated clothing and shoes and call a physician.
Inhalation
Immediately relocate self or casualty to fresh air. If breathing is difficult, give cardiopulmonary resuscitation (CPR). Avoid mouth-to-mouth resuscitation.

Ingestion
Wash out mouth with water; Do NOT induce vomiting; call 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).

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

5. FIRE FIGHTING MEASURES

5.1 Extinguishing media
Suitable extinguishing media
Use water spray, dry chemical, foam, and carbon dioxide fire extinguisher.

5.2 Special hazards arising from the substance or mixture
During combustion, may emit irritant fumes.

5.3 Advice for firefighters
Wear self-contained breathing apparatus and protective clothing.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures
Use full personal protective equipment. Avoid breathing vapors, mist, dust or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.
Refer to protective measures listed in sections 8.

6.2 Environmental precautions
Try to prevent further leakage or spillage. Keep the product away from drains or water courses.

6.3 Methods and materials for containment and cleaning up
Absorb solutions with finely-powdered liquid-binding material (diatomite, universal binders); Decontaminate surfaces and equipment by scrubbing with alcohol; Dispose of contaminated material according to Section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling
Avoid inhalation, contact with eyes and skin. Avoid dust and aerosol formation. Use only in areas with appropriate exhaust ventilation.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly sealed in cool, well-ventilated area. Keep away from direct sunlight and sources of ignition.
Recommended storage temperature: Powder -20°C 3 years
4°C 2 years
In solvent -80°C 6 months
-20°C 1 month
Shipping at room temperature if less than 2 weeks.

7.3 Specific end use(s)
No data available.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters
Components with workplace control parameters
This product contains no substances with occupational exposure limit values.

8.2 Exposure controls

Engineering controls
Ensure adequate ventilation. Provide accessible safety shower and eye wash station.

Personal protective equipment

- **Eye protection**: Safety goggles with side-shields.
- **Hand protection**: Protective gloves.
- **Skin and body protection**: Impervious clothing.
- **Respiratory protection**: Suitable respirator.
- **Environmental exposure controls**: Keep the product away from drains, water courses or the soil. Clean spillages in a safe way as soon as possible.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

- **Appearance**: Light yellow to yellow (Solid)
- **Odor**: No data available
- **Odor threshold**: No data available
- **pH**: No data available
- **Melting/freezing point**: No data available
- **Boiling point/range**: No data available
- **Flash point**: No data available
- **Evaporation rate**: No data available
- **Flammability (solid, gas)**: No data available
- **Upper/lower flammability or explosive limits**: No data available
- **Vapor pressure**: No data available
- **Vapor density**: No data available
- **Relative density**: No data available
- **Water Solubility**: No data available
- **Partition coefficient**: No data available
- **Auto-ignition temperature**: No data available
- **Decomposition temperature**: No data available
- **Viscosity**: No data available
- **Explosive properties**: No data available
- **Oxidizing properties**: No data available

9.2 Other safety information
No data available.

10. STABILITY AND REACTIVITY

10.1 Reactivity
No data available.

10.2 Chemical stability
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
10.4 Conditions to avoid
No data available.

10.5 Incompatible materials
Strong acids/alkalis, strong oxidising/reducing agents.

10.6 Hazardous decomposition products
Under fire conditions, may decompose and emit toxic fumes.
Other decomposition products - no data available.

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

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

Skin corrosion/irritation
Classified based on available data. For more details, see section 2

Serious eye damage/irritation
Classified based on available data. For more details, see section 2

Respiratory or skin sensitization
Classified based on available data. For more details, see section 2

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

Carcinogenicity
IARC: No component of this product present at a level equal to or greater than 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
ACGIH: No component of this product present at a level equal to or greater than 0.1% is identified as a potential or confirmed carcinogen by ACGIH.
NTP: No component of this product present at a level equal to or greater than 0.1% is identified as a anticipated or confirmed carcinogen by NTP.
OSHA: No component of this product present at a level equal to or greater than 0.1% is identified as a potential or confirmed carcinogen by OSHA.

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

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
PBT/vPvB assessment unavailable as chemical safety assessment not required or not conducted.

12.6 Other adverse effects
No data available.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods
Product
Dispose substance in accordance with prevailing country, federal, state and local regulations.

Contaminated packaging
Conduct recycling or disposal in accordance with prevailing country, federal, state and local regulations.

14. TRANSPORT INFORMATION

DOT (US)
This substance is considered to be non-hazardous for transport.

IMDG
This substance is considered to be non-hazardous for transport.

IATA
This substance is considered to be non-hazardous for transport.

15. REGULATORY INFORMATION

SARA 302 Components:
No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components:
This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards:
No SARA Hazards.

Massachusetts Right To Know Components:
No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components:
No components are subject to the Pennsylvania Right to Know Act.

New Jersey Right To Know Components:
No components are subject to the New Jersey Right to Know Act.

California Prop. 65 Components:
This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION
Copyright 2018 MedChemExpress. The above information is correct to the best of our present knowledge but does not purport to be all inclusive and should be used only as a guide. The product is for research use only and for experienced personnel. It must only be handled by suitably qualified experienced scientists in appropriately equipped and authorized facilities. The burden of safe use of this material rests entirely with the user. MedChemExpress disclaims all liability for any damage resulting from handling or from contact with this product.

Caution: Product has not been fully validated for medical applications. For research use only.

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