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

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Acute toxicity, oral (Category 4), H302
Skin corrosion/irritation (Category 2), H315
Serious eye damage/eye irritation (Category 2A), H319
Specific target organ toxicity, single exposure; Respiratory tract irritation (Category 3), H335

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal word Warning
Hazard statement(s)
H302 Harmful if swallowed
H315 Causes skin irritation
H319 Causes serious eye irritation
H335 May cause respiratory irritation
Precautionary statement(s)
Prevention
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

Response
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

2.3 Other hazards
None.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Formula: \( \text{C}_{21}\text{H}_{27}\text{ClN}_{8}\text{S} \)
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: -20°C, sealed storage, away from moisture
* In solvent: -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)
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
Solid
Odor
No data available
<table>
<thead>
<tr>
<th>Property</th>
<th>Information</th>
</tr>
</thead>
<tbody>
<tr>
<td>Odor threshold</td>
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<tr>
<td>pH</td>
<td>No data available</td>
</tr>
<tr>
<td>Melting/freezing point</td>
<td>No data available</td>
</tr>
<tr>
<td>Boiling point/range</td>
<td>No data available</td>
</tr>
<tr>
<td>Flash point</td>
<td>No data available</td>
</tr>
<tr>
<td>Evaporation rate</td>
<td>No data available</td>
</tr>
<tr>
<td>Flammability (solid, gas)</td>
<td>No data available</td>
</tr>
<tr>
<td>Upper/lower flammability or explosive limits</td>
<td>No data available</td>
</tr>
<tr>
<td>Vapor pressure</td>
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</tr>
<tr>
<td>Vapor density</td>
<td>No data available</td>
</tr>
<tr>
<td>Relative density</td>
<td>No data available</td>
</tr>
<tr>
<td>Water Solubility</td>
<td>No data available</td>
</tr>
<tr>
<td>Partition coefficient</td>
<td>No data available</td>
</tr>
<tr>
<td>Auto-ignition temperature</td>
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</tr>
<tr>
<td>Decomposition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>Viscosity</td>
<td>No data available</td>
</tr>
<tr>
<td>Explosive properties</td>
<td>No data available</td>
</tr>
<tr>
<td>Oxidizing properties</td>
<td>No data available</td>
</tr>
</tbody>
</table>

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
No data available.

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

**Additional information**
This information is based on our current knowledge. However the chemical, physical, and toxicological properties have not been completely investigated.

### 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)
Proper shipping name: Not dangerous goods
UN number: -
Class: -
Packing group: -

IMDG
Proper shipping name: Not dangerous goods
UN number: -
Class: -
Packing group: -

IATA
Proper shipping name: Not dangerous goods
UN number: -
Class: -
Packing group: -

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 anyother reproductive harm.

16. OTHER INFORMATION

Copyright 2023 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.