

Imidazole Ketone Erastin (IKE) SDS | MSDS

1.PRODUCT AND COMPANY IDENTIFICATION

Product identifier

- **Product Name:** Imidazole Ketone Erastin (IKE)
- **Catalog Number:** S8877
- **CAS Number:** 1801530-11-9
- **IUPAC Name:** 4(3H)-Quinazolinone, 2-[[4-[2-(4-chlorophenoxy)acetyl]-1-piperazinyl]methyl]-3-[5-[2-(1H-imidazol-1-yl)acetyl]-2-(1-methylethoxy)phenyl]-

Relevant identified uses and uses advised against

- **Identified uses:** For research and development use only; laboratory chemicals; manufacture of substances.
- **Uses advised against:** Not for pharmaceutical, household, or other unapproved uses.

Details of the supplier

- **Company :** Selleck Chemicals
- **TollFree :** +1 877 796-6397
- **Tel :** +1 832 582-8158
- **Fax :** +1 832 582-8590

Emergency telephone number

- **Emergency phone #:** +1 832 582-8158

2. HAZARDS IDENTIFICATION

GHS Classification:

Acute toxicity, Oral (Category 4)

Pictogram:



Signal Word: Warning

Hazard Statements:

H302: Harmful if swallowed.

Precautionary Statements:

- **Prevention:** P264: Wash skin thoroughly after handling. P270: Do not eat, drink or smoke when using this product.

- **Response:** P301 + P312 + P330: IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell. Rinse mouth.
- **Disposal:** P501: Dispose of contents/container to an approved waste disposal plant.

Other Hazards:

None known.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture: Mixture

Components:

- **Chemical Name:** 4(3H)-Quinazolinone, 2-[[4-[2-(4-chlorophenoxy)acetyl]-1-piperazinyl]methyl]-3-[5-[2-(1H-imidazol-1-yl)acetyl]-2-(1-methylethoxy)phenyl]-
- **CAS-No.:** 1801530-11-9
- **Concentration (% w/w):** >= 80 - <= 100% (Actual concentration withheld as a trade secret)

4. FIRST AID MEASURES

General Advice: Show this safety data sheet to the doctor in attendance.

If Inhaled: Move person into fresh air.

In Case of Skin Contact: Take off contaminated clothing immediately. Rinse skin with water/shower.

In Case of Eye Contact: Rinse out with plenty of water. Remove contact lenses.

If Swallowed: Immediately make victim drink water (maximum of two glasses). Consult a physician.

Most Important Symptoms and Effects: The most important known symptoms and effects are described in the labelling (Section 2) and/or in Section 11.

Protection of First-Aiders: Refer to Section 8 for personal protection.

Notes to Physician: N/A.

5. FIREFIGHTING MEASURES

Suitable Extinguishing Media: Water, Foam, Carbon dioxide (CO₂), Dry powder.

Unsuitable Extinguishing Media: No limitations of extinguishing agents are given for this substance/mixture.

Specific Hazards: Mixture contains combustible ingredients. Development of hazardous combustion gases or vapors is possible in the event of fire.

Hazardous Combustion Products: Carbon oxides, Nitrogen oxides (NO_x), Hydrogen chloride gas.

Specific Extinguishing Methods: N/A.

Further Information: Suppress gases/vapors/mists with water spray jet. Prevent fire extinguishing water from contaminating surface water or ground water systems.

Special Protective Equipment: In the event of fire, wear self-contained breathing apparatus.

6. ACCIDENTAL RELEASE MEASURES

Personal Precautions and Emergency Procedures:

- **For non-emergency personnel:** Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area and consult an expert.
- **For emergency responders:** Use personal protection as recommended in Section 8.

Environmental Precautions: Do not let product enter drains.

Methods and Materials for Containment and Cleaning Up: Cover drains. Collect, bind, and pump off spills. Observe material restrictions (Sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

7. HANDLING AND STORAGE

Precautions for Safe Handling: For precautions see section 2.2.

Conditions for Safe Storage: Keep container tightly closed in a dry place.

Storage Class: 11 (Combustible Solids).

Recommended Storage Temperature: -13 - 14 °F / -25 - -10 °C.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Control Parameters: Contains no substances with occupational exposure limit values.

Engineering Measures: N/A.

Personal Protective Equipment:

- **Respiratory Protection:** Required when dusts are generated. Recommended filter type: P2 (based on DIN EN 143, DIN 14387).
- **Eye Protection:** Use safety glasses tested and approved under government standards such as NIOSH (US) or EN 166 (EU).
- **Skin and Body Protection:** Wear protective clothing.
- **Hygiene Measures:** Change contaminated clothing. Preventive skin protection is recommended. Wash hands after working with the substance.

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance: powder

Color: N/A

Odor: N/A

Odor Threshold: N/A

pH: N/A

Melting Point: N/A

Boiling Point: N/A

Flash Point: N/A

Evaporation Rate: N/A

Flammability (solid, gas): N/A

Vapor Pressure: N/A

Relative Vapor Density: N/A

Relative Density: N/A

Density: N/A

Water Solubility: Soluble (68 °F / 20 °C)

Partition Coefficient (n-octanol/water): N/A

Autoignition Temperature: N/A

Decomposition Temperature: N/A

Viscosity: N/A

Explosive Properties: Not classified as explosive.

Oxidizing Properties: None

Molecular Weight: 655.14 g/mol

Particle Size: N/A

10. STABILITY AND REACTIVITY

Reactivity: Flammable organic substances in fine distribution may have dust explosion potential when whirled up.

Chemical Stability: Stable under standard ambient conditions (room temperature).

Possibility of Hazardous Reactions: Violent reactions possible with strong oxidizing agents.

Conditions to Avoid: No information available.

Incompatible Materials: Strong oxidizing agents.

Hazardous Decomposition Products: In the event of fire, see Section 5.

11. TOXICOLOGICAL INFORMATION

Acute Toxicity:

- **Oral:** Acute toxicity estimate Oral - 500.1 mg/kg (Expert judgment based on QSAR approach).
- **Inhalation:** N/A.
- **Dermal:** N/A.

Skin Corrosion/Irritation: N/A.

Serious Eye Damage/Irritation: N/A.

Respiratory or Skin Sensitization: N/A.

Germ Cell Mutagenicity: N/A.

Carcinogenicity:

- **IARC:** No component present at levels $\geq 0.1\%$ is identified as a probable, possible or confirmed human carcinogen.
- **NTP:** No component present at levels $\geq 0.1\%$ is identified as a known or anticipated carcinogen.

- **OSHA:** No component present at levels $\geq 0.1\%$ is on OSHA's list of regulated carcinogens.

Reproductive Toxicity: N/A.

STOT - Single Exposure: N/A.

STOT - Repeated Exposure: N/A.

Aspiration Hazard: N/A.

Additional Information: To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. Other dangerous properties cannot be excluded. Handle in accordance with good industrial hygiene and safety practice.

12. ECOLOGICAL INFORMATION

Ecotoxicity: N/A.

Persistence and Degradability: N/A.

Bioaccumulative Potential: N/A.

Mobility in Soil: N/A.

Other Adverse Effects: This product neither contains, nor was manufactured with a Class I or Class II ODS (Ozone-Depleting Substance) as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App. A + B).

13. DISPOSAL CONSIDERATIONS

Waste Treatment Methods: Waste material must be disposed of in accordance with national and local regulations. Leave chemicals in original containers. Do not mix with other waste. Handle uncleaned containers in the same manner as the product itself.

14. TRANSPORT INFORMATION

DOT (49 CFR): Not regulated as a dangerous good.

IATA: Not regulated as a dangerous good.

IMDG: Not regulated as a dangerous good.

Transport in Bulk: Not applicable for product as supplied.

Special Precautions: Not classified as dangerous in the meaning of transport regulations. Poison Inhalation Hazard: No.

15. REGULATORY INFORMATION

CERCLA Reportable Quantity: This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity: This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity: This material does not contain any components with a section 302 EHS TPQ.

SARA 313: 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.

Clean Air Act:

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCM Intermediate or Final VOC's (40 CFR 60.489).

Clean Water Act:

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

US State Regulations:

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

Maine Chemicals of High Concern: Product does not contain any listed chemicals

Vermont Chemicals of High Concern: Product does not contain any listed chemicals

Washington Chemicals of High Concern: Product does not contain any listed chemicals

The components of this product are reported in the following inventories:

TSCA: Product contains substance(s) not listed on TSCA inventory.

TSCA list:

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

16. OTHER INFORMATION

Revision Date: 2026/07/09

Further Information: The information provided is believed to be correct but is not exhaustive and should be used only as a guideline based on current knowledge. It does not represent a guarantee of the properties of the product. Selleck Chemicals Corporation and its Affiliates shall not be held liable for any damage resulting from handling or contact with the product.