

According to the federal final rule of hazard communication revised on 2012 (HazCom 2012)

Product Identification: Isonipecotic acid

0023Gj Ghs10 Div.3 sds Isonipecotic acid

Date of issue: March 29, 2024

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Supersedes version	: 0023Gj Ghs09 Div.3 sds Isonipecotic acid



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ECTION 1.:	IDENTIFICATION	
PRODUCT NAME	Isonipecotic acid	
CAS RN	498-94-2	
EC#	207-872-3	
SYNONYM	4-piperidinecarboxylic acid.4-Hexahydroisonicotinic acid.	
SYSTEMATIC NAME	4-piperidinecarboxylic acid. Isonipecotic acid.	
MOLECULAR FORMULA	$C_6H_{11}NO_2$	
STRUCTURAL FORMULA	ОН	
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1.3 Emergency telephone:

For Chemical Emergency ONLY (in the case of fire, leak, spill, exposure or accident) Call Chemtrec: 1-800-424-9300 (US), 1-703-527-3887 (Outside U.S.) Chemtrec (India) : 000-800-100-7141

For ALL other emergencies call Emergency Control Room Gajraula at 99970 22412

Product Uses:

• Isonipecotic Acid is used as an intermediate in the preparation of Active Pharmaceutical ingredients like Diphenoxylate, Meperidine and Phenoperidine.

SECTION 2:

HAZARDS IDENTIFICATION

GHS CLASSIFICATION

Skin corrosion / irritant: Category 2 Serious eye damage/eye irritation: Category 2A Specific target organ toxicity: Category 3 (After single exposure)



Hazard Pictogram: GHS 07 Signal Word: Warning!

HAZARD AND PRECAUTIONARY STATEMENTS:

HAZARD STATEMENTS

- H315: Causes skin irritation.
- H319: Causes serious eye irritation.
- H335: May cause respiratory irritation.

PRECAUTIONARY STATEMENTS

- P264: Wash hands thoroughly after handling.
- P280: Wear protective gloves/protective clothing/eye protection/face protection.
- P261: Avoid breathing dust/fume/gas/mist/vapors/spray.
- P271: Use only outdoors or in a well-ventilated area.
- P302+352: IF ON SKIN: Wash with plenty of soap and water.
- P332+313: If skin irritation occurs: Get medical advice/attention.
- P362: Take off contaminated clothing and wash before reuse.



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- P305+351+338: IF IN EYES: Rinse continuously with water for several minutes. Remove contact lenses if present and easy to do continue rinsing.
- P337+P313: If eye irritation persists: Get medical advice attention.
- P304+340: IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
- P312: Call a POISON CENTER or doctor/physician if you feel unwell.
- P403+233: Store in a well ventilated place. Keep container tightly closed.
- P405: Store locked up.
- P501: Dispose of contents/container to local/regional/national/international regulations.

SECTION 3:

COMPOSITION / INFORMATION ON INGERDIENTS

Sr.No.	Chemical	CAS #	EC#	Purity
1	Isonipecotic Acid	498-94-2	207-872-3	~98%

SECTION 4:

FIRST AID MEASURES

4.1. Description of first aid measures

- **Eyes**: If in eyes rinse cautiously with water for at least 15 minutes. Remove contact lenses if easy to do so. Continue rinsing. Seek medical attention.
- **Skin:** Immediately take off all contaminated clothing. Wash thoroughly with water for at least 15 minutes. Wash contaminated clothes before reuse. Seek immediate medical attention.
- **Inhalation**: Remove to fresh air and keep at rest in a position comfortable for breathing. Call a physician if you feel unwell.
- **Ingestion:** If swallowed call a poison center if you feel unwell. Rinse mouth. Do NOT induce vomiting by use of emetics. Seek medical attention.

4.2. Most important symptoms and effects, both acute and delayed Key symptoms

• Acute effects:

Isonipecotic acid is irritating to eyes and skin and respiratory system. It is irritating to mucous membranes and upper respiratory tract, it may cause irritation of the digestive tract system if swallowed. It may causes drowsiness or dizziness. Follow safe industrial hygiene practices and always wear proper protective equipment when handling this compound.

• Chronic effects:

Repeated or prolonged exposure to this compound is not known to aggravate existing medical conditions. **4.3. Indication of any immediate medical attention and special treatment needed**



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• Note to Physician: No specific indications. Treatment should be based on the judgment of the physician in response to the reactions of the patient

SECTION 5:

FIRE-FIGHTING MEASURES

Flash Point: Not available

Flammability: Non flammable

5.1 Extinguishing media:

• Appropriate extinguishing media: Dry chemical powder, carbon dioxide, and alcohol resistant foam. Water may also be used. Fight larger fire with water spray or alcohol resistant foam. Water can be effective in cooling down the fire-exposed containers and Knocking down the vapours. Water jets may be used to flush spills away and dilute the same to nonflammable mixtures fog or alcohol-resistant foam by directing streams to the periphery of the fires to prevent spread.

5.2 Special Protective Equipment and Precautions for Fire Fighter:

- Evacuate the area and fight fires from a safe distance.
- If tank, rail car or tank truck is involved in a fire, ISOLATE for 800 meters (1/2 mile) in all directions; also, consider initial evacuation for 800 meters (1/2 mile) in all directions or as per locally valid procedures.
- Fire fighters must wear Self Contained Breathing Apparatus (SCBA) and full protective clothing. The chemical is harmful in contact with skin.
- Report any run-off of fire waters contaminated with this chemical as per local and federal procedures applicable.

5.3 Unusual fire and explosion hazard:

- Toxic vapors may be released on thermal decomposition including nitrogen oxides, hydrogen chloride, carbon monoxide, Carbon di-oxide and cyanide.
- High vapor concentration may result in an explosion hazard.
- Vapors are heavier than air. May travel considerable distance from source and flashback.

SECTION 6 : ACCIDENTAL RELEASE MEASURES

Minor Spills

- Clean up all spills immediately following relevant Standard Operating Procedures.
- Avoid breathing vapors and contact with skin and eyes.
- Shut off leak source if possible.
- Shut off all possible sources of ignition.
- Wear protective clothing, boots, impervious gloves and safety glasses.
- Wipe up.

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• Decontaminate all equipment.

Major Spill

- Alert Emergency Responders and tell them location and nature of hazard.
- Shut off all possible sources of ignition and increase ventilation.
- Wear protective clothing, full boots, impervious gloves, safety glasses and Self Contained Breathing Apparatus (SCBA), as may be deemed appropriate.
- Clear area of personnel and move upwind.
- Stop leaks if possible.
- Prevent, by any means available, spillage from entering drains or water and watercourses.
- Collect recoverable product into labeled containers for recycling, recovery or disposal.
- Contain spill with sand, earth or vermiculite.
- Spread area with lime or absorbent material, and leave for at least 1 hour before washing.
- Clean up all tools and equipment.
- Inform authorities in event of contamination of any public sewers, drains or water bodies.

SECTION 7:

HANDLING AND STORAGE

7.1. Precautions for safe handling

- Do not breathe vapor or mist.
- Wear protective gloves/clothing and eye/face protection.
- Wash thoroughly after handling.
- Ground and secure containers when dispensing or pouring product.
- Avoid contact with incompatible materials.
- When handling, DO NOT eat, drink or smoke.
- Launder contaminated clothing before re-use.
- If on skin or hair, IMMEDIATELY remove all contaminated clothing and rinse/shower with plenty of water.
- Use in a well ventilated place/Use protective clothing commensurate with exposure levels.

7.2. Conditions for safe storage, including any incompatibilities

- Store at ambient temperature in a dry and well ventilated place
- Store away from incompatible materials
- Keep securely closed when not in use.
- Store locked up.



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SECTION 8 : EXPOSURE CONTROLS / PERSONAL PROTECTION

Control parameters

Exposure Limits Values

Chemical name	ACGIH TLV	OSHA PEL	NIOSH
Isonipecotic Act	id None listed	None listed	None listed

Exposure Limits (International):

• Not available.

Exposure controls

Appropriate Engineering Controls:

• Provide exhaust ventilation or other engineering controls to keep the relevant airborne concentrations below their respective occupational exposure limits. Local ventilation is usually preferred. Ensure that eyewash stations and safety showers are close to the workstation location.

Personal Protection:

- Protective clothing should be selected specifically for the working place, depending on concentration and quantity of the hazardous substances handled. The resistance of the protective clothing to chemicals should be ascertained with the respective supplier.
- Hands: Wear appropriate protective gloves to prevent skin exposure.
- **Eyes:** Safety goggles/ Chemical Safety glasses and Face shield.
- **Clothing:** Boots and clothing to prevent contact.
- **Respirator:** Follow the OSHA respirator regulations found in 29CFR 1910.134 or European Standard EN 149. Always use a NIOSH or European Standard EN 149 approved respirator when necessary. For emergency situations, wear a positive pressure, pressure-demand, full face piece self-contained breathing apparatus (SCBA) or pressure- demand supplied air respirator with escape SCBA and a fully-encapsulating, chemical resistant suit. (EPA,1998).

General Hygiene and general comments:

- Wash hands and face after working with substance.
- Immediately change contaminated clothing.
- Apply skin protective barrier cream.



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SECTION 9 : PHYSICAL AND CHEMICAL PROPERTIES

• Information on basic physical and chemical properties.

S.No	Parameter	Typical value
1.	Appearance	White powder
2.	Odor	Not available
3.	Odor Threshold	Not available
4.	Melting point	336°C
5.	Boiling point	Not available
6.	Flash point	Not available
7.	Evaporation rate (n-BuAc=1)	Not available
8.	Explosive limits	Not available
9.	Vapor pressure	Not available
10.	Vapor density (air=1)	Not available
11.	Specific gravity (water=1)	Not available
12.	Solubility	Freely soluble in water (292 g/l), Soluble in Dichloromethane
13.	pH	Not available
14.	Log Kow (octonol/water)	-3.05(Estimated)
15.	Auto-ignition temperature	Not available
16.	Decomposition temperature	Not available
17.	Viscosity	Not available
18.	Molecular Weight	129.16
19.	Flammability	Non Flammable
20.	Oxidizer	No
21.	Corrosive material	No
22.	Explosive material	No



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SECTION 10:

STABILITY AND REACTIVITY

- **Stability:** Stable under normal temperatures and pressures. Darkens at 300°C.
- **Conditions to avoid:** Keep away from heat, sparks, flame, high temperature and incompatible chemicals, dust generation. Not compatible with strong oxidizing agents.
- **Incompatible chemicals:** Strong Oxidizing Agents.
- **Hazardous decomposition products:** Thermal decomposition may produce carbon monoxide, Carbon dioxide and nitrogen oxide.
- Hazardous Polymerization: Has not been reported.

SECTION 11:

TOXICOLOGICAL INFORMATION

- a) Acute toxicity
- Isonipecotic acid is irritating to eyes and skin and respiratory system. It is irritating to mucous membranes and upper respiratory tract may cause irritation of the digestive tract system if swallowed. It may causes drowsiness or dizziness. Follow safe industrial hygiene practices and always wear proper protective equipment when handling this compound.

RTECS#: NS5150000 **LD50(Rat) Oral:** >5000 mg/kg

- b) Skin corrosion/irritation
 - Causes skin irritation.
- c) Serious eye damage/irritation
 - Causes serious eye irritation.
- d) Respiratory or skin sensitization
 - No data is available
- e) Germ cell Mutagenicity
 - No data is available.
- f) Carcinogenicity
 - Not listed by NTP, IARC and OSHA.
 - Not present on the EU CMR list.
 - According to information presently available Isonipecotic acid is not found to be carcinogenic.
- g) Reproductive toxicity
 - No data is available.
- h) STOT-single exposure
 - May cause respiratory irritation.



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i) STOT- repeated exposure

• No data available.

- j) Aspiration Hazards
 - No data available.

SECTION 12:

ECOLOGICAL INFORMATION

Toxicity :

Ecotoxicity (Estimated)

- Estimated LC50 (96 h) : 516000 mg/l Intermediate substance is not estimated to be toxic to fish (acute toxicity).
- Estimated Chronic Value : 180000 mg/L Intermediate substance is not estimated to be toxic to fish (Chronic toxicity).
- Estimated LC50 (48 h) :34000 mg/L Intermediate substance is not estimated to be toxic to aquatic invertebrates (acute toxicity).
- Estimated Chronic Value : 1580 mg/L Intermediate substance is not estimated to be toxic to aquatic invertebrates (chronic toxicity).
- Estimated EC50 (96h) : 90100 mg/L Estimated Chronic Value : 19500 mg/L

Intermediate substance is not estimated to be toxic to aquatic algae.

Persistence and degradability

• It is expected to be readily biodegradable in aerobic and anaerobic conditions. Therefore, Isonipecotic acid is estimated not to be persistent in the environment

Bio accumulative potential

- BCF = 3.16 l/kg wet wt. (BCF<500: No bioconcentration expected)
- Log Kow = -3.05

Based on the Log Kow and Bio concentration factor value it is expected to have negligible potential to concentrate in fatty tissue of fish and aquatic organisms relative to its surroundings. Isonipecotic acid is not expected to bio accumulate in the food chain because it does not exceed the BCF criteria

Mobility in soil

- Log Koc= 0.913 (estimated). Moderate sorption.
- Henry's Law Constant 6.43E-012 atm-m3/mole at 25 degrees. It is non-volatile from aqueous bodies.
- Log Kow= -3.05 (estimated). Negligible potential to bio accumulate.

Other adverse effects.

• Environment Fate:



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Based on the environmental modeling, this material has a moderate potential to get absorbed in the organic matter of soil and is non-volatile from water bodies. Since this is an estimated result it is recommended that the material should be disposed into the environment. The material should never be disposed into the sewage.

SECTION 13:

DISPOSAL CONSIDERATIONS

- Recycle to process, if possible. Consult your local regional authorities. You may be able to dissolve or mix material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber system. Observe all federal, state and local regulations when disposing of the substance.
- Note that disposal regulations may also apply to empty containers and equipment rinsates.

SECTION 14:

TRANSPORT INFORMATION

• This substance is considered to be Non Hazardous for transport by Air/Rail/Road and Sea and thus not regulated by IATA/ICAO/ARD/RID/IMO/IMDG.

Environmental hazards:

• Marine pollutant: No

SECTION 15:REGULATORY INFORMATIONClassification as per CLP Regulation 1272/2008:

- Hazards Class and Category: Skin Irrit Cat. 2; Eye Irrit Cat 2; STOT SE Cat. 3
- Hazard Statements: H315; H319; H335

Chemical Inventory Lists:	Status
TSCA:	Listed (Active)
EINECS:	207-872-3
Canada(DSL/NDSL):	Listed/NDSL
Japan:	5-770
Korea:	Not listed
Australia:	Not listed
China: IECSC	Listed
Philippines: PICCS	Listed
New Zealand (NZIoc)	Listed

US information



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CERCLA (Comprehensive Environmental Response, Compensation, and Liability Act): Isonipecotic acid is not listed

SARA 302/304 : Isonipecotic acid is not listed SARA 311/312 : See section 2 for more information California Prop. 65: Isonipecotic acid is not listed CAA (Clean Air Act): Isonipecotic acid is not listed CWA (Clean Water Act): Isonipecotic acid is not listed

EU Information

Water hazard class (WGK): WGK 3 (Severe hazards to water) Substance of Very High Concern (SVHC) according to the REACH Regulations (EC) No. 1907/2006: Isonipecotic acid is not listed

SECTION 16:

OTHER INFORMATION

Compilation information of safety data sheet Chemical: Isonipecotic acid CAS #: 498-94-2 File Name: 0023Gj Ghs10 Div.3 sds Isonipecotic acid Revision Number: 10 Date of Issue: March 29, 2024 Revision Due Date: February, 2027

(a) A key or legend to aberrations and acronyms used in the safety data sheet;

- PBT =Persistent Bio accumulative and Toxic.
- vPvB= Very Persistent and Very Bio accumulative.
- SCBA= Self Contained Breathing Apparatus.
- NIOSH REL= National Institute for Occupational Safety and Health Recommended Exposure Limit. OSHA PEL=Occupational Safety and Health Administration Permissible Exposure Limit.
- OELTWA= Occupational Exposure Limit Time Weighted Averages.
- IDLH= Immediately Dangerous to Life or Health.
- UEL= Upper Explosive Limit.
- LEL= Lower Explosive Limit.
- RTECS= Registry of Toxic Effects of Chemical Substances.
- NTP=National Toxicology Program.
- IARC= International Agency for Research on Cancer.
- EPA=Environmental Protection Agency.
- TSCA= Toxic Substances Control Act.
- CERCLA= Comprehensive Environmental Response, Compensation, and Liability Act.
- SARA= Superfund Amendments and Reauthorization Act.



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- NFPA= National Fire Protection Association.
- WHIMS= Workplace Hazardous Materials Information System.
- DSL/NDSL= Domestic/Non-Domestic Substances List.
- CSR=Chemical Safety Report.
- BCF = Bio Concentration Factor.
- DNEL = Derived No Effect Level.
- PNEC = Predicted No Effect Concentration.
- TLV = Threshold Limit Value.
- ACGIH = American Conference of Governmental Industrial Hygienists.
- REACH = Registration, Evaluation .Authorization and Restriction of Chemicals.
- CLP = Classification, Labeling and Packaging.
- LD / LC = Lethal Doses / Lethal Concentration.
- GHS = Globally Harmonized System.
- ADR = Accord europeen relative au transport international de marchandises.
- IMDG-Code = International Maritime Code for Dangerous Goods.
- EmS = Emergency measures on Sea.
- ICAO = International Civil Aviation Organization.
- IATA/DGR= International Air Transport Association/Dangerous Goods Regulation.

(b) Key Literature reference and sources for data

Biographical reference and data sources

- CLP REG (regulation) (EC) no. 1272/2008, last modification by regulation (EC) no. 790/2009
- DIR 67/548/EWG, last modification by DIR 2009/2/EC
- REG (EC) no. 1907/2006, last modification by REG (EC) Nr. 453/2009

Internet

• RTECS

Company's Declaration:

Information contained in this SDS is believed to be correct but no representation, guarantee or warranties of any kind are made as to its accuracy, suitability for a particular application or results to be obtained from them. This SDS shall be used as a guide only. Jubilant Ingrevia Limited makes no warranties expressed or implied of the adequacy of this document for any particular purpose.

(End of Safety Data Sheet)