

SAFETY DATA SHEET

Revision Date 29-Mar-2024

Revision Number 4

1. Identification

Product Name Isochroman

Cat No. : A12566

CAS No 493-05-0
Synonyms 3,4-Dihydro-1H-2-benzopyran

Recommended Use Laboratory chemicals.
Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-343-0660
Fax: 800-322-4757

Emergency Telephone Number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

2. Hazard(s) identification

Classification

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Flammable liquids

Category 4

Label Elements

Signal Word

Warning

Hazard Statements

Combustible liquid

Precautionary Statements

Prevention

Keep away from heat/sparks/open flames/hot surfaces. - No smoking

Wear protective gloves/protective clothing/eye protection/face protection

Fire

In case of fire: Use CO₂, dry chemical, or foam for extinction

Storage

Store in a well-ventilated place. Keep cool

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

None identified

3. Composition/Information on Ingredients

Component	CAS No	Weight %
Isochromane	493-05-0	99

4. First-aid measures

Eye Contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes.
Skin Contact	Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes.
Inhalation	Remove from exposure, lie down. Remove to fresh air.
Ingestion	Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Drink plenty of water. If possible drink milk afterwards.
Most important symptoms and effects	Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Water spray. Carbon dioxide (CO ₂). Dry chemical. Alcohol resistant foam. Water mist may be used to cool closed containers.
Unsuitable Extinguishing Media	No information available
Flash Point	65 °C / 149 °F
Method -	No information available
Autoignition Temperature	No information available
Explosion Limits	
Upper	No data available
Lower	No data available
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available

Specific Hazards Arising from the Chemical

Combustible material. Flammable. Containers may explode when heated.

Hazardous Combustion Products

Thermal decomposition can lead to release of irritating gases and vapors. Carbon monoxide (CO). Carbon dioxide (CO₂).

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full

protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

NFPA

Health
0

Flammability
1

Instability
0

Physical hazards
N/A

6. Accidental release measures

Personal Precautions

Remove all sources of ignition. Take precautionary measures against static discharges.

Environmental Precautions

See Section 12 for additional Ecological Information.

Methods for Containment and Clean Up

Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal. Sweep up and shovel into suitable containers for disposal. Remove all sources of ignition.

7. Handling and storage

Handling

Avoid contact with skin and eyes. Avoid contact with skin and clothing. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Avoid breathing vapors or mists. Do not ingest. If swallowed then seek immediate medical assistance. Wash thoroughly after handling. Keep away from open flames, hot surfaces and sources of ignition.

Storage.

Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Keep away from heat, sparks and flame. Keep containers tightly closed in a dry, cool and well-ventilated place. Incompatible Materials. Strong oxidizing agents.

8. Exposure controls / personal protection

Exposure Guidelines

This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.

Engineering Measures

None under normal use conditions. Ensure adequate ventilation, especially in confined areas.

Personal Protective Equipment**Eye/face Protection**

Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

Respiratory Protection

No protective equipment is needed under normal use conditions.

Recommended Filter type:

Particle filter.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State

Liquid

Appearance

Light yellow

Odor

Odorless

Odor Threshold

No information available

pH

No information available

Melting Point/Range

No data available

Boiling Point/Range

75 °C / 167 °F @ 4 MBAR

Flash Point

65 °C / 149 °F

Evaporation Rate	No information available
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	No information available
Vapor Density	4.63
Specific Gravity	1.060
Solubility	No information available
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	No information available
Decomposition Temperature	No information available
Viscosity	No information available
Molecular Formula	C9 H10 O
Molecular Weight	134.18

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Stable under normal conditions.
Conditions to Avoid	Incompatible products. Keep away from open flames, hot surfaces and sources of ignition.
Incompatible Materials	Strong oxidizing agents
Hazardous Decomposition Products	Thermal decomposition can lead to release of irritating gases and vapors, Carbon monoxide (CO), Carbon dioxide (CO ₂)
Hazardous Polymerization	No information available.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information No acute toxicity information is available for this product

Component Information
Toxicologically Synergistic Products No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation	No information available
Sensitization	No information available
Carcinogenicity	The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
Isochromane	493-05-0	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure None known

STOT - repeated exposure None known

Aspiration hazard	No information available
Symptoms / effects, both acute and delayed	Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting
Endocrine Disruptor Information	No information available
Other Adverse Effects	The toxicological properties have not been fully investigated.

12. Ecological information

Ecotoxicity

Do not empty into drains.

Persistence and Degradability Persistence is unlikely based on information available.

Bioaccumulation/ Accumulation No information available.

Mobility Will likely be mobile in the environment due to its volatility.

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT COMBUSTIBLE LIQUID, NOT REGULATED FOR TRANSPORT IN THIS QUANTITY
According to 49 CFR §173.150(f)(1), this material should be reclassified as NA1993, Combustible Liquid, NOS if it is shipped in bulk.

UN-No NA1993
Proper Shipping Name Combustible liquid, n.o.s.
Packing Group III

TDG Not regulated

IATA Not regulated

IMDG/IMO Not regulated

15. Regulatory information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Isochromane	493-05-0	-	-	-

Legend:

TSCA US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

'-' - Not Listed

TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT) Not applicable

TSCA 12(b) - Notices of Export Not applicable

International Inventories

Canada (DSL/NDL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
Isochromane	493-05-0	-	-	207-774-0	X	-		X	-	-

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

U.S. Federal Regulations

SARA 313

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372

SARA 311/312 Hazard Categories

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

CWA (Clean Water Act) Not applicable

Clean Air Act Not applicable

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA

This material, as supplied, does not contain any substances regulated as hazardous substances under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

California Proposition 65 This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations Not applicable

U.S. Department of Transportation

Reportable Quantity (RQ): N
DOT Marine Pollutant N
DOT Severe Marine Pollutant N

U.S. Department of Homeland Security This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade No information available

Authorisation/Restrictions according to EU REACH Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Isochromane	493-05-0	-	-	-

Safety, health and environmental regulations/legislation specific for the substance or mixture

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
Isochromane	493-05-0	Not applicable	Not applicable	Not applicable	Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Other International Regulations

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
Isochromane	493-05-0	Not applicable	Not applicable	Not applicable	Not applicable

16. Other information

Prepared By

Health, Safety and Environmental Department
Email: chem.techinfo@thermofisher.com
www.thermofisher.com

Revision Date

29-Mar-2024

Print Date

29-Mar-2024

Revision Summary

New emergency telephone response service provider.

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of SDS