

• SAFETY DATA SHEET

Version 6.7
Revision Date 12/23/2025
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : Isobutyl 1,2-dihydro-2-isobutoxy-1-quinolinecarboxylate

Product Number : 178241
Brand : Aldrich
Index-No. : 613-281-00-5
CAS-No. : 38428-14-7

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Hazards for the product as supplied

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Germ cell mutagenicity : Category 2
Carcinogenicity : Category 1B

Other hazards

None known.

GHS label elements

Hazard pictograms :



Signal word : Danger

Hazard statements : H341 Suspected of causing genetic defects.
H350 May cause cancer.

Precautionary statements : **Prevention:**
P201 Obtain special instructions before use.
P202 Do not handle until all safety precautions have been read and understood.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
Response:
P308 + P313 IF exposed or concerned: Get medical advice/ attention.
Storage:
P405 Store locked up.
Disposal:
P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance
CAS-No. : 38428-14-7

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
quinoline	91-22-5*	>= 0.5 - <= 1.5	TSC

* Indicates that the identifier is a CAS No.

TSC- the actual concentration or concentration range is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice	: Show this safety data sheet to the doctor in attendance.
If inhaled	: After inhalation: fresh air. Call in physician.
In case of skin contact	: In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.
In case of eye contact	: After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.
If swallowed	: After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.
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) and/or in section 11
Protection of first-aiders	: For personal protection see section 8.
Notes to physician	: No data available

SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media	: Water Foam Carbon dioxide (CO ₂) Dry powder
Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	: Combustible.

Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

Hazardous combustion products	: Carbon oxides Nitrogen oxides (NOx)
Specific extinguishing methods	: No data available
Further information	: Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.
Special protective equipment for fire-fighters	: Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures	: Advice for non-emergency personnel: Do not breathe vapours, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert. Advice for emergency responders: For personal protection see 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 possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on safe handling : Work under hood. Do not inhale substance/mixture.
Avoid generation of vapours/aerosols.

Further information on storage conditions : Tightly closed.
Keep in a well-ventilated place.
Keep locked up or in an area accessible only to qualified or authorised persons.

Storage class : 6.1C, Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

Recommended storage temperature : Recommended storage temperature see product label.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
quinoline	91-22-5	TWA	0.001 ppm	US WEEL

Biological occupational exposure limits

Components	CAS-No.	Control parameters	Biological specimen	Sampling time	Permissible concentration	Basis
quinoline	91-22-5	1-Hydroxypyrene	Urine	End of shift at end of workweek	2.5 µg/l	ACGIH BEI

Engineering measures : No data available

Personal protective equipment

Respiratory protection : required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: : Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Hand protection

Remarks : required

Eye protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
Safety glasses

Skin and body protection : protective clothing

Hygiene measures : Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : viscous

Color : colourless

Odor : No data available

Odor Threshold : No data available

pH : No data available

Melting point : No data available

Boiling point/boiling range : 284 - 288 °F / 140 - 142 °C (0.3 hPa)

Flash point : 235 °F / 113 °C

Method: closed cup

Evaporation rate : No data available

Flammability (solid, gas) : No data available

Flammability (liquids) : No data available

Burning rate : No data available

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Upper explosion limit / Upper flammability limit	: No data available
Lower explosion limit / Lower flammability limit	: No data available
Vapor pressure	: No data available
Relative vapour density	: No data available
Relative density	: No data available
Density	: 1.022 g/mL (77 °F / 25 °C)
Water solubility	: No data available
Partition coefficient: n- octanol/water	: No data available
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available
Molecular weight	: 303.40 g/mol
Particle characteristics Particle size	: No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	: Forms explosive mixtures with air on intense heating. A range from approx. 15 Kelvin below the flash point is to be rated as critical.
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .

Possibility of hazardous reactions : No data available

Conditions to avoid : Strong heating.

Incompatible materials : acids

Hazardous decomposition products : In the event of fire: see section 5

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

Acute toxicity estimate Oral - > 5,000 mg/kg
(Calculation method)
LD50 Oral - Rat - male and female - 262 mg/kg (quinoline)
(OECD Test Guideline 401)
Symptoms: Nausea, Vomiting, Gastrointestinal disturbance
Inhalation: No data available
Symptoms: Possible damages:, mucosal irritations
Acute toxicity estimate Dermal - > 5,000 mg/kg
(Calculation method)
LD50 Dermal - Rat - male and female - 1,377 mg/kg (quinoline)
(OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit (quinoline)
Result: irritating - 24 h
(Draize Test)
Remarks: (ECHA)

Serious eye damage/eye irritation

Eyes - Rabbit (quinoline)
Result: Severe irritations - 24 h
Remarks: (ECHA)

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse (quinoline)
Result: negative
(OECD Test Guideline 429)

Germ cell mutagenicity

Evidence of genetic defects.
Suspected of causing genetic defects. (quinoline)
Test Type: Mutagenicity (mammal cell test): chromosome aberration.
(quinoline)
Test system: Chinese hamster ovary cells
Metabolic activation: with and without metabolic activation
Result: Positive results were obtained in some in vitro tests.
Remarks: (ECHA)
Test Type: Ames test
(quinoline)
Test system: Salmonella typhimurium

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Metabolic activation: with and without metabolic activation
Method: Mutagenicity (Salmonella typhimurium - reverse mutation assay)
Result: Positive results were obtained in some in vitro tests.
Remarks: (ECHA)
Test Type: sister chromatid exchange assay
(quinoline)
Test system: Chinese hamster ovary cells
Metabolic activation: with and without metabolic activation
Result: Positive results were obtained in some in vitro tests.
Remarks: (ECHA)
Test Type: In vitro mammalian cell gene mutation test
(quinoline)
Test system: Mouse lymphoma test
Metabolic activation: without metabolic activation
Result: positive
Remarks: (ECHA)
(quinoline)
Test Type: Micronucleus test
Species: Mouse
Cell type: Bone marrow
Application Route: Intraperitoneal injection

Result: positive
Remarks: (ECHA)

Carcinogenicity

Possible carcinogen.

Presumed to have carcinogenic potential for humans (quinoline)

IARC: 2B - Group 2B: Possibly carcinogenic to humans (quinoline)

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

Effects due to ingestion may include:, Liver injury may occur. (quinoline)

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. (quinoline)

After absorption:

(quinoline)
Possible symptoms:
(quinoline)
Fever
muscle twitching
Dizziness
Convulsions
(quinoline)
Absorption may result in damage of the following:
(quinoline)
Liver
Kidney
Central nervous system
(quinoline)
Other dangerous properties can not be excluded.
(quinoline)
This substance should be handled with particular care.
(quinoline)
Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence
(quinoline)

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

quinoline:

Toxicity to fish	: LC50 (Poecilia reticulata (guppy)): 29.9 mg/l End point: mortality Exposure time: 96 h Test Type: semi-static test Analytical monitoring: yes Method: OECD Test Guideline 203
Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)	: NOEC (Daphnia magna (Water flea)): 0.8 mg/l End point: reproduction rate Exposure time: 21 d Test Type: semi-static test Analytical monitoring: yes Remarks: (ECHA)
Toxicity to microorganisms	: EC50 (activated sludge): 243 mg/l Exposure time: 3 h Test Type: static test Method: OECD Test Guideline 209 GLP: yes

Ecotoxicology Assessment

Chronic aquatic toxicity : Toxic to aquatic life with long lasting effects.

Persistence and degradability

Components:

quinoline:

Biodegradability : Result: Readily biodegradable.
Biodegradation: 100 %
Exposure time: 49 d
Method: OECD Test Guideline 301D

Bioaccumulative potential

Components:

quinoline:

Bioaccumulation : Species: Cyprinus carpio (Carp)
Bioconcentration factor (BCF): 1.6 - 2.5
Exposure time: 6 Weeks
Temperature: 77 °F / 25 °C
Concentration: 0.8 mg/l
Elimination: yes

Partition coefficient: n-octanol/water : log Pow: 2.03
Method: OECD Test Guideline 107
Remarks: Bioaccumulation is not expected.
(Lit.)

Mobility in soil

No data available

Other adverse effects

Components:

quinoline:

Additional ecological information : Discharge into the environment must be avoided.

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

Not regulated as a dangerous good

IMDG-Code

Not regulated as a dangerous good

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR Road

Not regulated as a dangerous good

Poison Inhalation Hazard : No

Special precautions for user

Remarks : Not classified as dangerous in the meaning of transport regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
quinoline	91-22-5	5000	

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 311/312 Hazards : Acute Health Hazard
Chronic Health Hazard

SARA 313 : The following components are subject to reporting levels established by SARA Title III, Section 313:

quinoline 91-22-5 >= 1 - < 5 %

Clean Water Act

The following Hazardous Substances are listed under the U.S. CleanWater Act, Section 311, Table 116.4A:

quinoline 91-22-5 >= 1 - < 5 %

The following Hazardous Chemicals are listed under the U.S. CleanWater Act, Section 311, Table 117.3:

quinoline 91-22-5 $\geq 1 - < 5 \%$
This product contains the following toxic pollutants listed under the U.S. Clean Water Act Section 307

quinoline 91-22-5 $\geq 1 - < 5 \%$
This product does not contain any priority pollutants related to the U.S. Clean Water Act

US State Regulations

Massachusetts Right To Know

quinoline 91-22-5

Pennsylvania Right To Know

quinoline 91-22-5

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

California Prop. 65

WARNING: This product can expose you to chemicals including quinoline, which is/are known to the State of California to cause cancer. For more information go to www.P65Warnings.ca.gov.

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.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

ACGIH BEI : ACGIH - Biological Exposure Indices (BEI)
US WEEL : USA. Workplace Environmental Exposure Levels (WEEL)
US WEEL / TWA : 8-hr TWA

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response;

EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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