

SAFETY DATA SHEET

Version 6.3
Revision Date 02/07/2023
Print Date 12/02/2023

SECTION 1: Identification of the substance/mixture and of the company/undertaking**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

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

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

SECTION 2: Hazards identification**2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Germ cell mutagenicity (Category 2), H341
Carcinogenicity (Category 1B), H350

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Danger

Hazard statement(s)	
H341	Suspected of causing genetic defects.
H350	May cause cancer.
Precautionary statement(s)	
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.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.1 Substances

Formula	: C ₁₈ H ₂₅ NO ₃
Molecular weight	: 303.40 g/mol
CAS-No.	: 38428-14-7
EC-No.	: 202-051-6
Index-No.	: 613-281-00-5

Component	Classification	Concentration
quinoline		
	Acute Tox. 3; Acute Tox. 4; Skin Irrit. 2; Eye Irrit. 2A; Muta. 2; Carc. 1B; Aquatic Acute 3; Aquatic Chronic 2; H301, H312, H315, H319, H341, H350, H402, H411	>= 1 - < 5 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Show this material 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.

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) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures**5.1 Extinguishing media****Suitable extinguishing media**

Water Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO_x)

Combustible.

Vapors 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.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures**6.1 Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 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.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Hygiene measures

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

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage class

Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
quinoline	91-22-5	TWA	0.001 ppm	USA. Workplace Environmental Exposure Levels (WEEL)
	Remarks	Skin		

8.2 Exposure controls

Appropriate engineering controls

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

Personal protective equipment

Eye/face protection

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

Skin protection

required

Body Protection

protective clothing

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.

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance	Form: clear, viscous, liquid Color: colorless
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	No data available
f) Initial boiling point and boiling range	140 - 142 °C 284 - 288 °F at 0.3 hPa
g) Flash point	113 °C (235 °F) - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	No data available
l) Vapor density	No data available
m) Density	1.022 g/mL at 25 °C (77 °F)
Relative density	No data available
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Autoignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 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.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Strong heating.

10.5 Incompatible materials

acids

10.6 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

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

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

Presumed to have carcinogenic potential for humans (quinoline)

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

NTP: No ingredient 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)

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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

12.1 Toxicity

Toxicity to fish	semi-static test LC50 - <i>Poecilia reticulata</i> (guppy) - 29.9 mg/l - 96 h (quinoline) (OECD Test Guideline 203)
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Toxicity to bacteria

Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	semi-static test NOEC - <i>Daphnia magna</i> (Water flea) - 0.8 mg/l - 21 d (quinoline) Remarks: (ECHA)
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12.2 Persistence and degradability

Biodegradability	Result: 100 % - Readily biodegradable. (OECD Test Guideline 301D)
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12.3 Bioaccumulative potential

Bioaccumulation	Cyprinus carpio (Carp) - 6 Weeks at 25 °C - 0.8 mg/l(quinoline) Bioconcentration factor (BCF): 1.6 - 2.5 Elimination: yes
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12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

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. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

DOT (US)

Not dangerous goods

IMDG

Not dangerous goods

IATA

Not dangerous goods

Further information

Not classified as dangerous in the meaning of transport regulations.

SECTION 15: Regulatory information

SARA 302 Components

This material does not contain any components with a section 302 EHS TPQ.

SARA 313 Components

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

	CAS-No.	Revision Date
quinoline	91-22-5	2007-07-01

SARA 311/312 Hazards

Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
quinoline	91-22-5	2007-07-01

Pennsylvania Right To Know Components

quinoline

CAS-No.
91-22-5Revision Date
2007-07-01**California Prop. 65 Components**

, which is/are known to the State of California to
cause cancer. For more information go to
www.P65Warnings.ca.gov/quinoline

CAS-No.
91-22-5Revision Date
2013-12-20

SECTION 16: Other information**Further information**

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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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