

Chemical Safety Data Sheet MSDS / SDS

Isobutyl 1,2-dihydro-2-isobutoxy-1-quinoline-carboxylate

Revision Date:2023-11-29 Revision Number:1

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

Product identifier

Product name : Isobutyl 1,2-dihydro-2-isobutoxy-1-quinoline-carboxylate
CBnumber : CB6224549
CAS : 38428-14-7
EINECS Number : 253-925-9
Synonyms : IIDQ,1-Isobutoxycarbonyl-2-isobutoxy-1,2-dihydroquinoline

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 400-158-6606

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

Precautionary statements

P308+P313 IF exposed or concerned: Get medical advice/attention.

P201 Obtain special instructions before use.

Hazard statements

H350 May cause cancer

H341 Suspected of causing genetic defects

SECTION 3: Composition/information on ingredients

Substance

Product name	: Isobutyl 1,2-dihydro-2-isobutoxy-1-quinoline-carboxylate
Synonyms	: IIDQ, 1-Isobutoxycarbonyl-2-isobutoxy-1,2-dihydroquinoline
CAS	: 38428-14-7
EC number	: 253-925-9
MF	: C18H25NO3
MW	: 303.4

SECTION 4: First aid measures

Description of first aid measures

General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. 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

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Special hazards arising from the substance or mixture

Carbon oxides Nitrogen oxides (NOx)

Advice for firefighters

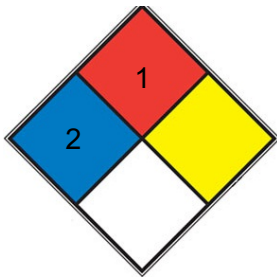
Wear self-contained breathing apparatus for firefighting if necessary.

Further information

No data available

NFPA 704

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HEALTH 2 Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

FIRE 1 Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

REACT

SPEC.

HAZ.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

For personal protection see section 8.

Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

Methods and materials for containment and cleaning up

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

Advice on safe handling

Avoid exposure - obtain special instructions before use. **Advice on safe handling**

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

Hygiene measures

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Storage conditions

Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

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

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

Exposure controls

Personal protective equipment

Eye/face protection

Safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full- face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance colorless clear, viscous, liquid

Odour No data available

Odour Threshold	No data available
pH	No data available
Melting point/freezing point	No data available
Initial boiling point and boiling range	140 - 142 °C at 0,3 hPa
Flash point	113 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	No data available
Vapour density	No data available
Relative density	1,022 g/mL at 25 °C No data available
Water solubility	No data available
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
Explosive properties	No data available
Oxidizing properties	No data available

Other safety information

No data available

SECTION 10: Stability and reactivity

Reactivity

No data available

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

No data available

Conditions to avoid

No data available

Incompatible materials

acids

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

Acute toxicity estimate Oral - > 2.000 mg/kg

(Calculation method)

LD50 Oral - Rat - male and female - 262 mg/kg (quinoline) (OECD Test Guideline 401)

Symptoms: Nausea, Vomiting, Gastrointestinal disturbance Symptoms: Possible damages:, mucosal irritations

Acute toxicity estimate Dermal - > 2.000 mg/kg (Calculation method)

LD50 Dermal - Rat - male and female - 1.377 mg/kg (quinoline) (OECD Test Guideline 402)

Skin corrosion/irritation

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

No data available

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

SECTION 12: Ecological information

Toxicity**Toxicity to fish**

semi-static test LC50 - *Poecilia reticulata* (guppy) - 29,9 mg/l - 96 h (quinoline)

(OECD Test Guideline 203)

Toxicity to bacteria**Persistence and degradability**

Biodegradability Result: 100 % - Readily biodegradable.

(OECD Test Guideline 301D)

Bioaccumulative potential

Bioaccumulation *Cyprinus carpio* (Carp) - 6 Weeks

at 25 °C - 0,8 mg/l(quinoline)

Mobility in soil

No data available

Bioconcentration factor (BCF): 1,6 - 2,5 Elimination: yes

Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Other adverse effects

Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

Waste treatment methods**Product**

Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

UN number

ADR/RID: - IMDG: - IATA: -

UN proper shipping name

ADR/RID: Not dangerous goods IMDG: Not dangerous goods

IATA: Not dangerous goods

14.3 Transport hazard class(es)

ADR/RID: - IMDG: - IATA: -

Packaging group

14.4

ADR/RID: - IMDG: - IATA: -

Environmental hazards

14.5

ADR/RID: no IMDG Marine pollutant: no IATA: no

14.6 Special precautions for user

Further information

Not classified as dangerous in the meaning of transport regulations.

SECTION 15: Regulatory information

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

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: <https://www.mem.gov.cn/>

Measures for Environmental Management of New Chemical Substances

Vietnam National Chemical Inventory:Not Listed. website: <https://chemicaldata.gov.vn/>

United States Toxic Substances Control Act (TSCA) Inventory:Not Listed. website: <https://www.epa.gov/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Not Listed. website: <https://emb.gov.ph/>

New Zealand Inventory of Chemicals (NZIoC):Not Listed. website: <https://www.epa.govt.nz/>

Korea Existing Chemicals List (KECL):Not Listed. website: <http://ncis.nier.go.kr>

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: <https://www.mee.gov.cn/>

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: <https://echa.europa.eu/>

EC Inventory:Listed.

SECTION 16: Other information

Abbreviations and acronyms

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

STEL: Short term exposure limit

TWA: Time Weighted Average

References

- 【1】 CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- 【2】 ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- 【3】 ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>
- 【4】 eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:
http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
- 【5】 ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- 【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- 【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- 【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- 【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- 【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

Disclaimer:

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