

## Chemical Safety Data Sheet MSDS / SDS

**2-Isopropyl-5-methyl-2-hexenal**

Revision Date:2024-12-21 Revision Number:1

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

Product name : 2-Isopropyl-5-methyl-2-hexenal  
CBnumber : CB7238284  
CAS : 35158-25-9  
EINECS Number : 252-406-4  
Synonyms : 2-Isopropyl-5-methylhex-2-enal, 2-Isopropyl-5-methyl-2-hexenal

**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

Warning

**Precautionary statements**

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continuerinsing.

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

**Hazard statements**

H335 May cause respiratory irritation

H319 Causes serious eye irritation

H315 Causes skin irritation

H226 Flammable liquid and vapour

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## SECTION 3: Composition/information on ingredients

### Substance

Product name	: 2-Isopropyl-5-methyl-2-hexenal
Synonyms	: 2-Isopropyl-5-methylhex-2-enal, 2-Isopropyl-5-methyl-2-hexenal
CAS	: 35158-25-9
EC number	: 252-406-4
MF	: C <sub>10</sub> H <sub>18</sub> O
MW	: 154.25

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## SECTION 4: First aid measures

### Description of first aid measures

#### General advice

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

#### If inhaled

After inhalation: fresh air.

#### 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

### Indication of any immediate medical attention and special treatment needed

No data available

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## SECTION 5: Firefighting measures

### Extinguishing media

#### Suitable extinguishing media

Foam Carbon dioxide (CO<sub>2</sub>) Dry powder

#### Unsuitable extinguishing media

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

### Special hazards arising from the substance or mixture

Carbon oxides 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.

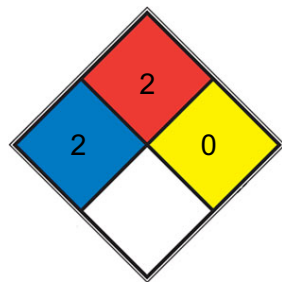
### Advice for firefighters

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

### Further information

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

### NFPA 704



☒ 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 2 Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, [sulfur](#))

☒ REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N<sub>2</sub>](#))

☐ SPEC.  
☐ HAZ.

## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition.

Evacuate the danger area, observe emergency procedures, consult an expert. 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 with liquid-absorbent material (e.g. Chemizorb? ). Dispose of properly. Clean up affected area.

### Reference to other sections

For disposal see section 13.

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## SECTION 7: Handling and storage

### Precautions for safe handling

#### Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

#### Hygiene measures

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

For precautions see section 2.2.

#### Conditions for safe storage, including any incompatibilities

#### Storage conditions

Tightly closed.

#### Specific end use(s)

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

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## 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

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.

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.

Do not let product enter drains.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Appearance	colorless liquid
Odour	characteristic
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	No data available
Initial boiling point and boiling range	189 °C - lit.
Flash point	63 °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	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

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## 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

Strong oxidizing agents

### Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - male and female - 6.800 mg/kg Remarks: (ECHA)

The value is given in analogy to the following substances: Citral Inhalation

LD50 Dermal - Rat - male and female - > 2.000 mg/kg Remarks: (ECHA)

The value is given in analogy to the following substances: Citral

#### Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin. Remarks: (ECHA)

The value is given in analogy to the following substances: Citral

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye irritation. (OECD Test Guideline 405)

The value is given in analogy to the following substances: Citral

#### Respiratory or skin sensitization

(OECD Test Guideline 406)

The value is given in analogy to the following substances: Citral

#### Germ cell mutagenicity

Test Type: Ames test

Test system: S. typhimurium

Metabolic activation: with and without metabolic activation Method: OECD Test Guideline 471

Result: negative

The value is given in analogy to the following substances: CitralTest Type: gene mutation test

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation Method: OECD Test Guideline 476

Result: negative

The value is given in analogy to the following substances: CitralTest Type: Chromosome aberration test in vitro

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation Method: OECD Test Guideline 473

Result: negative

The value is given in analogy to the following substances: Citral Test Type: Micronucleus test

Species: Mouse

Application Route: Oral

Method: OECD Test Guideline 474 Result: negative

The value is given in analogy to the following substances: Citral

#### **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

#### **toxicity**

Both the acute oral LD<sub>50</sub> value in rats and the acute dermal LD<sub>50</sub> value in rabbits exceeded 5 g/kg

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## SECTION 12: Ecological information

### **Toxicity**

#### **Toxicity to fish**

static test LC<sub>50</sub> - Leuciscus idus (Golden orfe) - 6,78 mg/l - 96 h (DIN 38412)

#### **Toxicity to daphnia and other aquatic invertebrates**

static test EC<sub>50</sub> - Daphnia magna (Water flea) - 6,8 mg/l - 48 h Remarks: (ECHA)

The value is given in analogy to the following substances: Citral

#### **Toxicity to algae**

static test ErC<sub>50</sub> - Desmodesmus subspicatus (green algae) - 103,8 mg/l - 72 h

Remarks: (ECHA)

The value is given in analogy to the following substances: Citral

#### **Toxicity to bacteria**

static test EC<sub>50</sub> - activated sludge - ca. 160 mg/l - 30 min (OECD Test Guideline 209)

### **Persistence and degradability**

No data available

### **Bioaccumulative potential**

No data available

### **Mobility in soil**

No data available

## 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

No data available

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## SECTION 13: Disposal considerations

### Waste treatment methods

### Product

See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## 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

### Transport hazard class(es)

ADR/RID: - IMDG: - IATA: -

### Packaging group

ADR/RID: - IMDG: - IATA: -

### Environmental hazards

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

### Special precautions for user

No data available

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## 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/>

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



United States Toxic Substances Control Act (TSCA) Inventory: Listed. website: <https://www.epa.gov/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS): Listed. website: <https://emb.gov.ph/>

New Zealand Inventory of Chemicals (NZIoC): Listed. website: <https://www.epa.govt.nz/>

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

EC Inventory: Listed.

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC): Listed. website: <https://www.mee.gov.cn/>

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## 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](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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