

Chemical Safety Data Sheet MSDS / SDS

2-Isopropyl-5-methyl-2-hexenal

Revision Date:2025-02-01 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

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 ₁₀ H ₁₈ O
MW	: 154.25

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

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing media

Foam Carbon dioxide (CO₂) 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.

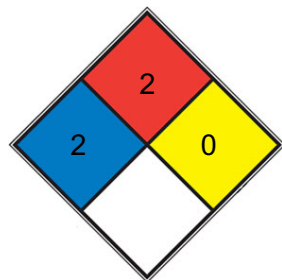
Advice for firefighters

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, [N2](#))

☐ 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.

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

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.

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

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

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 LD₅₀ value in rats and the acute dermal LD₅₀ value in rabbits exceeded 5 g/kg

SECTION 12: Ecological information

Toxicity

Toxicity to fish

static test LC₅₀ - Leuciscus idus (Golden orfe) - 6,78 mg/l - 96 h (DIN 38412)

Toxicity to daphnia and other aquatic invertebrates

static test EC₅₀ - 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 ErC₅₀ - 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 EC₅₀ - 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

SECTION 13: Disposal considerations

Waste treatment methods

Product

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

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

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/>

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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