



Safety Data Sheet

Section 1. Identification of the substance/mixture and of the company/undertaking

Product identifier:

Product name: 2,6-Dimethyl-4-heptanone

SDS No. : 2235E-3

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

Research and Development

Details of the supplier of the safety data sheet

Manufacturer/Supplier: KISHIDA CHEMICAL CO., LTD.

Address: 3-1, Honmachibashi, Chuo-ku, Osaka, JAPAN

Division: Chemical Safety Management Department

Telephone number: +81-6-6946-8061

FAX: +81-6-6946-1607

Section 2. Hazards identification

GHS classification and label elements of the product

Classification of the substance or mixture

PHYSICAL AND CHEMICAL HAZARDS

Flammable liquids: Category 3

HEALTH HAZARDS

Serious eye damage/eye irritation: Category 2B

Carcinogenicity: Category 1B

Specific target organ toxicity – single exposure: Category 1 (liver, central nervous system)

Specific target organ toxicity – single exposure: Category 3 (Respiratory tract irritation)

Specific target organ toxicity – single exposure: Category 3 (Narcotic effects)

Specific target organ toxicity – repeated exposure: Category 2 (central nervous system, respiratory system)

ENVIRONMENT HAZARDS

Hazardous to the aquatic environment, short-term (acute): Category 3

Hazardous to the aquatic environment, long-term (chronic): Category 3

(Note) GHS classification without description: Not classified/Classification not possible

Label elements



Signal word: Danger

HAZARD STATEMENT

Flammable liquid and vapor

Causes eye irritation

May cause cancer

Causes damage to organs (liver, central nervous system)

May cause respiratory irritation

May cause drowsiness or dizziness

May cause damage to organs through prolonged or repeated exposure (central nervous system, respiratory system)

Harmful to aquatic life with long lasting effects

PRECAUTIONARY STATEMENT

Prevention



Avoid release to the environment.

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Keep container tightly closed.

Ground and bond container and receiving equipment.

Use explosion-proof electrical/ventilating/lighting equipment.

Use non-sparking tools.

Take action to prevent static discharges.

Do not breathe dust/fume/gas/mist/vapors/spray.

Use only outdoors or in a well-ventilated area.

Wash contaminated parts thoroughly after handling.

Wear protective gloves/protective clothing/eye protection/face protection.

Do not eat, drink or smoke when using this product.

Response

In case of fire: Use appropriate media to extinguish.

Get medical advice/attention if you feel unwell.

IF exposed or concerned: Get medical advice/attention.

IF INHALED: Remove person to fresh air and keep comfortable for breathing.

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

If eye irritation persists: Get medical advice/attention.

Storage

Store in a well-ventilated place. Keep container tightly closed. Keep cool.

Disposal

Dispose of contents/container in accordance with local/national regulation.

Specific Physical and Chemical hazards

Flammable liquid. Vapor/air mixture may explode.

Section 3. Composition/information on ingredients

Mixture/Substance selection:

Substance

Ingredient name: 2,6-Dimethyl-4-heptanone

Content (%): 70 (min)

Chemical formula: CC(C)CC(=O)CC(C)C

Chemicals No, Japan: 2-2475

CAS No.: 108-83-8

MW: 142.24

ECNO: 203-620-1

Note: The figures shown above are not the specifications of the product.

Impurities

1,3,5-Trimethylbenzene 1.2% (CAS No. 108-67-8)

4-Methyl-2-pentanone 0.20% (CAS No. 108-10-1)

Section 4. First-aid measures

Descriptions of first-aid measures

General measures

Get medical advice/attention if you feel unwell.

IF INHALED

Remove person to fresh air and keep comfortable for breathing.

Call a POISON CENTER/doctor/physician if you feel unwell.

**IF ON SKIN (or hair)**

Take off immediately all contaminated clothing. Rinse skin with water or shower.

If skin irritation or rash occurs: Get medical advice/attention.

IF IN EYES

Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

If eye irritation persists: Get medical advice/attention.

IF SWALLOWED

Rinse mouth.

Call a POISON CENTER/doctor/physician if you feel unwell.

Section 5. Fire-fighting measures**Extinguishing media****Suitable extinguishing media**

In case of fire, use foam, dry powder, CO2 to extinguish.

Unsuitable extinguishing media

Indoor firefighting equipment or outdoor firefighting equipment

Sprinkler equipment

Dry-powder firefighting equipment – other (except for phosphate etc., hydrogen carbonate etc.)

Straight stream water extinguisher

Water mist extinguisher

Reinforcing liquid jet extinguisher

Dry-powder extinguisher – other (except for phosphate etc., hydrogen carbonate etc.)

Bucket of water or tank of water

Specific hazards arising from the substance or mixture

Containers may explode when heated.

Fire may produce irritating, corrosive and/or toxic gases.

Advice for firefighters**Specific fire-fighting measures**

Evacuate non-essential personnel to safe area.

Special protective equipment and precautions for fire-fighters

Wear fire resistant or flame retardant clothing.

Wear protective gloves/protective clothing/eye protection/face protection.

Firefighters should wear self-contained breathing apparatus with full face piece operated positive pressure mode.

Section 6. Accidental release measures**Personnel precautions, protective equipment and emergency procedures**

Ventilate area until material pick up is complete.

Wear proper protective equipment.

Environmental precautions

Prevent spills from entering sewers, watercourses or low areas.

Methods and materials for containment and cleaning up

Absorb spill with inert material (dry sand, earth, et al), then place in a chemical waste container.

Preventive measures for secondary accident

Collect spillage.



Section 7. Handling and storage

Precautions for safe handling

Preventive measures

(Exposure Control for handling personnel)

Do not breathe dust/fume/gas/mist/vapors/spray.

(Protective measures against fire and explosion)

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Ground and bond container and receiving equipment.

Use explosion-proof electrical/ventilating/lighting equipment.

Use non-sparking tools.

Take action to prevent static discharges.

(Exhaust/ventilator)

Exhaust/ventilator should be available.

(Safety treatments)

Avoid contact with skin.

Avoid contact with eyes.

Safety Measures

Use only outdoors or in a well-ventilated area.

Wear protective gloves/protective clothing/eye protection/face protection.

When using do not eat, drink or smoke.

Any incompatibilities

See "10.Stability and Reactivity"

Advice on general occupational hygiene

Wash contaminated parts thoroughly after handling.

Do not eat, drink or smoke when using this product.

Storage

Conditions for safe storage

Keep container tightly closed.

Store in a cool, dry place. Do not store in direct sunlight.

Container and packaging materials for safe handling

Glass

Polyethylene

Section 8. Exposure controls/personal protection

Control parameters

Adopted value

(2,6-Dimethyl-4-heptanone)

ACGIH(1979) TWA: 25ppm (URT & eye irr)

(1,3,5-Trimethylbenzene)

ACGIH(2021) TWA: 10ppm (CNS impair; hematologic eff)

(4-Methyl-2-pentanone)

ACGIH(2010) TWA: 20ppm;

STEL: 75ppm (URT irr; dizziness; headache)

OSHA-PEL

(2,6-Dimethyl-4-heptanone)

TWA: 50ppm, 290mg/m³

(4-Methyl-2-pentanone)

TWA: 100ppm, 410mg/m³

Exposure controls

Appropriate engineering controls

Do not use in areas without adequate ventilation.



Eye wash station should be available.
Washing facilities should be available.
Individual protection measures
Respiratory protection
Wear respiratory protection.
Hand protection
Wear protective gloves.
Eye protection
Wear eye/face protection.

Section 9. Physical and Chemical Properties

Information on basic physical and chemical properties

Physical state: Liquid
Color: Colorless, clear
Odor: Characteristic odor
Melting point/Freezing point: -42°C
Boiling point or initial boiling point: (2,6-Dimethyl-4-heptanone) 168°C
Boiling range data is not available.
Flammability (gases, liquids and solids) data is not available.
Lower and upper explosion limit/flammability limit:
Lower explosion limit: (93°C) 0.8 vol %
Upper explosion limit: (93°C) 6.2 vol %
Flash point: (2,6-Dimethyl-4-heptanone) 49°C
Auto-ignition temperature: (2,6-Dimethyl-4-heptanone) 396°C
Decomposition temperature data is not available.
pH data is not available.
Kinematic viscosity data is not available.
Solubility:
Solubility in water: None
n-Octanol/water partition coefficient data is not available.
Vapor pressure: 0.23 kPa (20°C)
Density and/or relative density: 0.81
Relative vapor density (Air=1): 4.9
Relative density of the Vapor/air – mixture at 20°C (Air = 1): 1.01
Particle characteristics data is not available.

Section 10. Stability and Reactivity

Reactivity
Not available.
Chemical stability
Stable under normal storage/handling conditions.
Possibility of hazardous reactions
Reacts with oxidants. Attacks some forms of plastic. (ICSC 0713)
Conditions to avoid
Contact with incompatible materials.
Contact with fire source.
Incompatible materials
Oxidizing agents
Hazardous decomposition products
Carbon oxides

Section 11. Toxicological Information

Information on toxicological effects

Acute toxicity

Acute toxicity (Oral)

[Data for components of the product]

[GHS Cat. Japan, base data]

(1,3,5-Trimethylbenzene)

rat LD50=4300-8642mg/kg (NITE Initial Risk Assessment Report, 2008)

(4-Methyl-2-pentanone)

rat LD50=2080mg/kg (ACGIH, 2010)

Acute toxicity (Inhalation)

[Data for components of the product]

[GHS Cat. Japan, base data]

(1,3,5-Trimethylbenzene)

mist: rat LC50=4800ppm/4hr (24mg/L/4hr) (MOE Result of the initial environmental risk assessment of chemicals, 2013)

(4-Methyl-2-pentanone)

vapor: rat LC50=8.2mg/L/4hr (NTP TR 538, 2007)

Irritant properties

Skin corrosion/irritation

[Data for components of the product]

[GHS Cat. Japan, base data]

(1,3,5-Trimethylbenzene)

rabbit (OECD TG 404) moderate to severe irritation (NITE Initial Risk Assessment Report, 2008)

Serious eye damage/irritation

[Data for components of the product]

[GHS Cat. Japan, base data]

(2,6-Dimethyl-4-heptanone)

rabbit recover after 7 days (SIDS, 2004)

(1,3,5-Trimethylbenzene)

rabbit mild irritation (NITE Initial Risk Assessment Report, 2008)

(4-Methyl-2-pentanone)

rabbit recover within 7 days (ECETOC TR48, 1992)

Allergenic and sensitizing effects data is not available.

Mutagenic effects data is not available.

Carcinogenicity

[Data for components of the product]

[GHS Cat. Japan, base data]

(4-Methyl-2-pentanone)

cat.1B; (IARC 101, 2012)

[IARC]

(4-Methyl-2-pentanone)

Group 2B : Possibly carcinogenic to humans

[ACGIH]

(4-Methyl-2-pentanone)

A3(2010) : Confirmed Animal Carcinogen with Unknown Relevance to Humans

[EU]

(4-Methyl-2-pentanone)

Category 2; Substances suspected human carcinogens

Reproductive toxicity data is not available.

Specific target organ toxicity (STOT)

STOT-single exposure

[Data for components of the product]

[cat.1]

[GHS Cat. Japan, base data]

(2,6-Dimethyl-4-heptanone)

liver, central nervous system (PATTY 6th, 2012)

[cat.3 (respiratory tract irritation)]

[GHS Cat. Japan, base data]

(2,6-Dimethyl-4-heptanone)

respiratory tract irritation (PATTY 6th, 2012)

(1,3,5-Trimethylbenzene)

respiratory tract irritation (MOE Result of the initial environmental risk assessment of chemicals, 2013)

(4-Methyl-2-pentanone)

respiratory tract irritation (PATTY 6th, 2012)

[cat.3 (narcotic effects)]

[GHS Cat. Japan, base data]

(2,6-Dimethyl-4-heptanone)

narcotic effect (PATTY 6th, 2012)

(1,3,5-Trimethylbenzene)

narcotic effect (MOE Result of the initial environmental risk assessment of chemicals, 2013)

(4-Methyl-2-pentanone)

narcotic effect (PATTY 6th, 2012)

STOT-repeated exposure

[Data for components of the product]

[cat.1]

[GHS Cat. Japan, base data]

(1,3,5-Trimethylbenzene)

central nervous system, respiratory system (MOE Result of the initial environmental risk assessment of chemicals, 2013)

Aspiration hazard

[Data for components of the product]

[cat.1]

[GHS Cat. Japan, base data]

(1,3,5-Trimethylbenzene)

cat. 1; hydrocarbon, kinematic viscosity=0.843 mm²/s (20°C), 0.630 mm²/s (50°C) (REACH Registration dossier, Accessed July 2021)

Section 12. Ecological Information

Toxicity

Aquatic toxicity

[Data for components of the product]

Hazardous to the aquatic environment, short-term (acute)

[GHS Cat. Japan, base data]

(2,6-Dimethyl-4-heptanone)

Crustacea (Brine shrimp) LC50=65mg/L/24hr (SIDS, 2004)

(1,3,5-Trimethylbenzene)

Crustacea (Daphnia magna) EC50=6mg/L/48hr; Fish (Carassius auratus) LC50=12.5mg/L/96hr (NITE Initial Risk Assessment Report, 2008)

(4-Methyl-2-pentanone)

Fish (Pimephales promelas) LC50=505mg/L/96hr (ECETOC TR91, 2003)

Hazardous to the aquatic environment, long-term (chronic)

[GHS Cat. Japan, base data]



(1,3,5-Trimethylbenzene)

Crustacea (Daphnia magna) NOEC=0.4mg/L/21days (SIAP, 2012)

(4-Methyl-2-pentanone)

Fish (Pimephales promelas) NOEC=57mg/L/31days (MOE Japan, 2008)

Water solubility

(2,6-Dimethyl-4-heptanone)

0.264 g/100 ml (PHYSPROP_DB, 2005)

(1,3,5-Trimethylbenzene)

very poor (ICSC, 2002)

(4-Methyl-2-pentanone)

1.91g/100 ml (20°C) (ICSC, 1997)

Persistence and degradability

[Data for components of the product]

(2,6-Dimethyl-4-heptanone)

Not rapidly degradable (BIOWIN)

(1,3,5-Trimethylbenzene)

Not rapidly degradable (BOD_Degradation : 0%/14 days (METI Existing Chemical Substances Safety Inspections Data, 1980))

(4-Methyl-2-pentanone)

Rapidly degradable (BOD_Degradation : 84%/14 days; TOC_Degradation: 97.1%/14 days;

GC_Degradation: 100%/14 days (MITI official bulletin))

Bioaccumulative potential

[Data for components of the product]

(1,3,5-Trimethylbenzene)

log Pow=3.42 (ICSC, 2002); BCF=342 (Check & Review, Japan)

(4-Methyl-2-pentanone)

log Pow=1.38 (ICSC, 1997)

Mobility in soil

Mobility in soil data is not available.

Other adverse effects

Ozone depleting chemical data is not available.

Section 13. Disposal considerations

Description of waste residues and information on their safe handling and methods of disposal, including the disposal of any contaminated packaging

Waste treatment methods

Avoid release to the environment.

Dispose of contents/container in accordance with local/national regulation.

Section 14. Transport Information

UN Number or ID Number : 1157

UN Proper Shipping Name :

DIISOBUTYL KETONE

Class or division (Transport hazard class) : 3

Packing group : III

ERG GUIDE No.: 128

IMDG Code (International Maritime Dangerous Goods Regulations)

UN Number or ID Number : 1157

UN Proper Shipping Name :

DIISOBUTYL KETONE

Class or division (Transport hazard class) : 3

Packing group : III

**IATA (Dangerous Goods Regulations)**

UN Number or ID Number : 1157

UN Proper Shipping Name :

DIISOBUTYL KETONE

Class or division (Transport hazard class) : 3

Hazard labels : Flamm.liquid

Packing group : III

Environmental hazards

Marine pollutants (yes/no) : no

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Noxious Liquid Substances ; Cat. X

1,3,5-Trimethylbenzene

Noxious Liquid Substances ; Cat. Y

2,6-Dimethyl-4-heptanone

Noxious Liquid Substances ; Cat. Z

4-Methyl-2-pentanone

Section 15. Regulatory Information

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

U.S. Toxic Substances Control Act (TSCA) Inventory

Chemicals listed in TSCA Inventory

4-Methyl-2-pentanone; 1,3,5-Trimethylbenzene; 2,6-Dimethyl-4-heptanone

Other regulatory information

Ensure this material in compliance with federal requirements and ensure conformity to local regulations.

Section 16. Other information**GHS classification and labelling**

Flammable liquids, Category 3: H226 Flammable liquid and vapour

Serious eye damage/eye irritation, Category 2B: H320 Causes eye irritation

Carcinogenicity, Category 1B: H350 May cause cancer

STOT – single exposure, Category 1: H370 Causes damage to organs

STOT – single exposure, Category 3, Respiratory tract irritation: H335 May cause respiratory irritation.

STOT – single exposure, Category 3, Narcotic effects: H336 May cause drowsiness or dizziness.

STOT – Repeated exposure, Category 2: H373 May cause damage to organs through prolonged or repeated exposure

Hazardous to the aquatic environment, short-term (acute), Category 3: H402 Harmful to aquatic life

Hazardous to the aquatic environment, long-term (chronic), Category 3: H412 Harmful to aquatic life with long lasting effects

References and sources for data

Globally Harmonized System of classification and labelling of chemicals, UN

Recommendations on the TRANSPORT OF DANGEROUS GOODS 21th edit., 2019 UN

IMDG Code, 2020 Edition (Incorporating Amendment 40-20)

IATA Dangerous Goods Regulations (62nd Edition) 2021

2020 EMERGENCY RESPONSE GUIDEBOOK (US DOT)

2022 TLVs and BEIs. (ACGIH)

Supplier's data/information

General Disclaimer

This data sheet was created based on the information we currently have and may be revised



according to new information. In addition, the precautions apply only to normal handling, and in the case of special handling, please make adequate countermeasure to maintain your safety.

The data given here is based on current knowledge and experience. The purpose of this Safety Data Sheet is to describe the products in terms of their safety requirements. The data does not signify any warranty with regard to the products' properties.

The GHS classification data given here is based on current Japan official data (NITE published in 2021).