

Chemical Safety Data Sheet MSDS / SDS

2,6-Dimethyl-4-heptanone

Revision Date:2026-06-27 Revision Number:1

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

Product name : 2,6-Dimethyl-4-heptanone
CBnumber : CB8852764
CAS : 108-83-8
EINECS Number : 203-620-1
Synonyms : DIBK,Diisobutyl Ketone

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 : 010-86108875

SECTION 2: Hazards identification**GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Warning

Precautionary statements

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.
P233 Keep container tightly closed.
P240 Ground/bond container and receiving equipment.
P241 Use explosion-proof electrical/ventilating/lighting/.../equipment.
P242 Use only non-sparking tools.
P243 Take precautionary measures against static discharge.

Hazard statements

H335 May cause respiratory irritation
H226 Flammable liquid and vapour

SECTION 3: Composition/information on ingredients

Substance

Product name	: 2,6-Dimethyl-4-heptanone
Synonyms	: DIBK, Diisobutyl Ketone
CAS	: 108-83-8
EC number	: 203-620-1
MF	: C ₉ H ₁₈ O
MW	: 142.24

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.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

In case of eye contact

After eye contact: rinse out with plenty of water. 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) 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

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

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

Development of hazardous combustion gases or vapours possible in the event of fire.

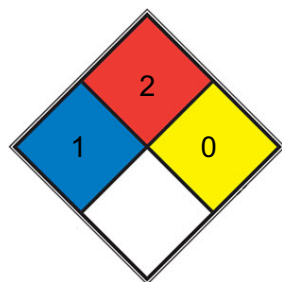
5.3 Advice for firefighters

In the event of fire, wear self-contained breathing apparatus.

5.4 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 1 Exposure would cause irritation with only minor residual injury (e.g. [acetone](#), sodium bromate, potassium chloride)

Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely

■ FIRE 2 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

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. Keep away from heat and sources of ignition.

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. Risk of explosion.

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 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 protection against fire and explosion

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

Hygiene measures

Change contaminated clothing. Wash hands after working with substance.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Storage class

Storage class (TRGS 510): 3: Flammable liquids

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

8.2 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

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.

Splash contact

Material: butyl-rubber

Minimum layer thickness: 0,3 mm

Break through time: 60 min

Material tested: Butoject® (KCL 897 / Aldrich Z677647, Size M) data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved

gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Flame retardant antistatic 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.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

a) Physical state	liquid
b) Color	colorless
c) Odor	Sweet Pineapple-Banana-like fruity taste, but with a somewhat harsh chemical note.
d) Melting point/freezing point	No data available
e) Initial boiling point and boiling range	165 - 170 °C - lit.
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	0.8-6.2%, 100°F
h) Flash point	49 °C - closed cup
i) Autoignition temperature	No data available
j) Decomposition temperature	No data available
k) pH	No data available
l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
m) Water solubility	0.05 g/100 mL
n) Partition coefficient n-octanol/water	No data available
o) Vapor pressure	1.7 mm Hg (20 °C)
p) Density	0,808 g/mL at 25 °C - lit.
Relative density	0.808 g/mL at 25 °C(lit.)
q) Relative vapor density	4.9 (vs air)
r) Particle characteristics	No data available
s) Explosive properties	Not classified as explosive.
t) Oxidizing properties	none
Solubility	Miscible with ethanol, ether, carbon tetrachloride, chloroform, benzene and most organic liquids.

Henry's Law Constant 6.36(x 10⁻⁴ atmm³/mol) at 20 °C (approximate - calculated from water solubility and vapor pressure)

Dielectric constant 9.910000000000001

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapor/air-mixtures are explosive at intense warming.

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

Heating.

10.5 Incompatible materials

Strong bases, Strong oxidizing agents, Strong acids, Strong reducing agents

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture Acute toxicity

Oral: No data available

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:; damage of respiratory tract

Dermal: No data available

Skin corrosion/irritation

Classified based on available data. For more details, see section 2

Serious eye damage/eye irritation

Classified based on available data. For more details, see section 2

Respiratory or skin sensitization

Classified based on available data. For more details, see section 2

Germ cell mutagenicity

Classified based on available data. For more details, see section 2

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

Mixture may cause respiratory irritation.

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

11.2 Additional Information

Endocrine disrupting properties

Product:

Assessment : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Hazardous properties cannot be excluded but are unlikely when the product is handled appropriately.

Components 2,6-Dimethylheptan-4-one

Acute toxicity

LD50 Oral - Rat - male and female - > 2.000 mg/kg (OECD Test Guideline 401)

LC50 Inhalation - Rat - 4 h - > 14,5 mg/l (OECD Test Guideline 403)

LD50 Dermal - Rat - male and female - > 2.000 mg/kg (OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h (OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation (OECD Test Guideline 405)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: Does not cause skin sensitization.

(OECD Test Guideline 406)

Germ cell mutagenicity

Classified based on available data. For more details, see section 2

Test Type: Ames test

Test system: *S. typhimurium*

Result: negative

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

Classified based on available data. For more details, see section 2

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

3,3,5-trimethylcyclohexanone

Acute toxicity

LD50 Oral - Rat - male and female - > 2.000 mg/kg (OECD Test Guideline 401)

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

LC50 Inhalation - Rat - male - 4 h - 14,2 mg/l - aerosol (OECD Test Guideline 403)

Symptoms: Shortness of breath, Cough, mucosal irritations, Possible damages:, damage of respiratory tract

Inhalation: absorption

LD50 Dermal - Rat - male and female - > 2.000 mg/kg (OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation (OECD Test Guideline 404)

Serious eye damage/eye irritation

Classified based on available data. For more details, see section 2

Respiratory or skin sensitization

Buehler Test - Guinea pig

Result: negative (OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster lung cells

Result: negative

Method: OECD Test Guideline 474

Species: Mouse - male and female

Result: negative

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

May cause respiratory irritation.

Acute oral toxicity - Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

Acute inhalation toxicity - Shortness of breath, Cough, mucosal irritations, Possible damages:, damage of respiratory tract

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

SECTION 12: Ecological information

12.1 Toxicity

Mixture

No data available

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 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.

12.6 Endocrine disrupting properties

Product:

Assessment : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission

Delegated regulation (EU) 2017/2100 or Commission

Regulation (EU) 2018/605 at levels of 0.1% or higher.

12.7 Other adverse effects

No data available

Components 2,6-Dimethylheptan-4-one

Toxicity to fish flow-through test LC50 - *Oncorhynchus mykiss* (rainbow trout) - 30 mg/l - 96 h (OECD Test Guideline 203)

Toxicity to daphnia Immobilization EC50 - *Daphnia magna* (Water flea) - 37,2 mg/l and other aquatic - 48 h invertebrates (OECD Test Guideline 202)

Toxicity to algae Growth inhibition EC50 - *Pseudokirchneriella subcapitata* (green algae) - 46,9 mg/l - 72 h (OECD Test Guideline 201)

3,3,5-trimethylcyclohexanone

Toxicity to fish static test LC50 - *Danio rerio* (zebra fish) - > 100 mg/l - 96 h (OECD Test Guideline 203)

Toxicity to daphnia static test EC50 - *Daphnia magna* (Water flea) - 180 mg/l - 48 and other aquatic h invertebrates (OECD Test Guideline 202)

Toxicity to algae static test ErC50 - *Desmodesmus subspicatus* (green algae) - > 82,27 mg/l - 72 h (OECD Test Guideline 201) static test

NOEC - *Desmodesmus subspicatus* (green algae) - > 82,27 mg/l - 72 h (OECD Test Guideline 201)

Toxicity to bacteria static test EC50 - activated sludge - 755 mg/l - 3 h (OECD Test Guideline 209)

SECTION 13: Disposal considerations

13.1 Waste treatment methods

No data available

SECTION 14: Transport information

14.1 UN number

ADR/RID: 1157

IMDG: 1157

IATA: 1157

14.2 UN proper shipping name

ADR/RID: DIISOBUTYL KETONE

IMDG: DIISOBUTYL KETONE

IATA: Diisobutyl ketone

14.3 Transport hazard class(es)

ADR/RID: 3

IMDG: 3

IATA: 3

14.4 Packaging group

ADR/RID: III

IMDG: III

IATA: III

14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

14.6 Special precautions for user

Tunnel restriction code : (D/E)

Further information : No data available

14.7 Maritime transport in bulk according to IMO instruments

Not applicable for product as supplied.

SECTION 15: Regulatory information

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

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

National legislation

Seveso III: Directive 2012/18/EU of the P5c FLAMMABLE LIQUIDS

European Parliament and of the Council on the control of major-accident hazards involving dangerous substances.

Other regulations

Take note of Dir 94/33/EC on the protection of young people at work.

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways

ADR - Agreement concerning the International Carriage of Dangerous Goods by Road

AIRC - Australian Inventory of Industrial Chemicals

ASTM - American Society for the Testing of Materials

bw - Body weight

CMR - Carcinogen, Mutagen or Reproductive Toxicant

DIN - Standard of the German Institute for Standardisation

DSL - Domestic Substances List (Canada)

EC_x - Concentration associated with x% response

EL_x - Loading rate associated with x% response

EmS - Emergency Schedule

ENCS - Existing and New Chemical Substances (Japan)

ErC_x - Concentration associated with x% growth rate response

GHS - Globally Harmonized System

GLP - Good Laboratory Practice

IARC - International Agency for Research on Cancer

IATA - International Air Transport Association

IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk

IC₅₀ - Half maximal inhibitory concentration

ICAO - International Civil Aviation Organization

IECSC - Inventory of Existing Chemical Substances in China

IMDG - International Maritime Dangerous Goods

IMO - International Maritime Organization

ISHL - Industrial Safety and Health Law (Japan)

ISO - International Organisation for Standardization

KECI - Korea Existing Chemicals Inventory

LC₅₀ - Lethal Concentration to 50 % of a test population

LD₅₀ - Lethal Dose to 50% of a test population (Median Lethal Dose)

MARPOL - International Convention for the Prevention of Pollution from Ships

n.o.s. - Not Otherwise Specified

NO(A)EC - No Observed (Adverse) Effect Concentration

NO(A)EL - No Observed (Adverse) Effect Level

NOELR - No Observable Effect Loading Rate

NZIoC - New Zealand Inventory of Chemicals

OECD - Organization for Economic Co-operation and Development

OPPTS - Office of Chemical Safety and Pollution Prevention

PBT - Persistent, Bioaccumulative and Toxic substance

PICCS - Philippines Inventory of Chemicals and Chemical Substances

(Q)SAR - (Quantitative) Structure Activity Relationship

REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals

RID - Regulations concerning the International Carriage of Dangerous Goods by Rail

SADT - Self-Accelerating Decomposition Temperature

SDS - Safety Data Sheet

TCSI - Taiwan Chemical Substance Inventory

TECI - Thailand Existing Chemicals Inventory

TSCA - Toxic Substances Control Act (United States)

UN - United Nations

UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods

vPvB - Very Persistent and Very Bioaccumulative

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.