

## Safety Data Sheet

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

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830 Issue date: 28-02-2023 Version: 1.0

### 1.1. Product identifier

Product form : Substance

: 2,6-DIMETHYL-4-HEPTANONE Trade name

EC Index-No. : 606-005-00-X EC-No. : 203-620-1 CAS-No. : 108-83-8 Product code : 03404

Type of product : flavouring ingredient

Formula C9H18O

Chemical structure

CH<sub>3</sub> O

Synonyms : Di-iso-butyl ketone, Isovalerone, 2,6-Dimethyl heptan-4-one

### 1.2. Relevant identified uses of the substance or mixture and uses advised against

#### 1.2.1. Relevant identified uses

Use of the substance/mixture : Laboratory chemicals

Manufacture of substances

#### 1.2.2. Uses advised against

No additional information available

#### 1.3. Details of the supplier of the safety data sheet

LOBA CHEMIE PVT.LTD.

107 Wode House Road, Jehangir Villa, Colaba

400005 Mumbai

INDIA

T +91 22 6663 6663 - F +91 22 6663 6699

info@lobachemie.com - www.lobachemie.com

### 1.4. Emergency telephone number

: +91 22 6663 6663 (9:00am - 6:00 pm) **Emergency number** 

## **SECTION 2: Hazards identification**

## 2.1. Classification of the substance or mixture

#### Classification according to Regulation (EC) No. 1272/2008 [CLP]

Flammable liquids, Category 3 H226 Specific target organ toxicity - Single exposure, Category 3, Respiratory H335

tract irritation

Full text of H- and EUH-statements: see section 16

## Adverse physicochemical, human health and environmental effects

Flammable liquid and vapour. May cause respiratory irritation.

## 2.2. Label elements

### Labelling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP)



GHS02

GHS07

Signal word (CLP) : Warning

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Hazard statements (CLP) : H226 - Flammable liquid and vapour.

H335 - May cause respiratory irritation.

Precautionary statements (CLP) : P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources.

No smoking.

P233 - Keep container tightly closed.

P240 - Ground and bond container and receiving equipment.
P241 - Use explosion-proof electrical/ventilating/lighting equipment.

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

P304+P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing.

### 2.3. Other hazards

No additional information available

## **SECTION 3: Composition/information on ingredients**

#### 3.1. Substances

Substance type : Mono-constituent

Name	Product identifier	%
2,6-DIMETHYL-4-HEPTANONE	CAS-No.: 108-83-8 EC-No.: 203-620-1 EC Index-No.: 606-005-00-X	100

#### 3.2. Mixtures

Not applicable

#### **SECTION 4: First aid measures**

#### 4.1. Description of first aid measures

First-aid measures general : Call a poison center or a doctor if you feel unwell.

First-aid measures after inhalation : Remove person to fresh air and keep comfortable for breathing. Call a poison center or a

doctor if you feel unwell.

First-aid measures after skin contact : Rinse skin with water/shower. Take off immediately all contaminated clothing.

First-aid measures after eye contact : Rinse eyes with water as a precaution.

First-aid measures after ingestion : Call a poison center or a doctor if you feel unwell.

### 4.2. Most important symptoms and effects, both acute and delayed

Symptoms/effects after inhalation : May cause respiratory irritation.

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

Treat symptomatically.

## **SECTION 5: Firefighting measures**

## 5.1. Extinguishing media

Suitable extinguishing media : Water spray. Dry powder. Foam. Carbon dioxide.

#### 5.2. Special hazards arising from the substance or mixture

Fire hazard : Flammable liquid and vapour. Hazardous decomposition products in case of fire : Toxic fumes may be released.

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#### 5.3. Advice for firefighters

Protection during firefighting

: Do not attempt to take action without suitable protective equipment. Self-contained breathing apparatus. Complete protective clothing.

#### **SECTION 6: Accidental release measures**

#### 6.1. Personal precautions, protective equipment and emergency procedures

#### 6.1.1. For non-emergency personnel

**Emergency procedures** 

: Ventilate spillage area. No open flames, no sparks, and no smoking. Avoid breathing dust/fume/gas/mist/vapours/spray.

6.1.2. For emergency responders

Protective equipment

: Do not attempt to take action without suitable protective equipment. For further information refer to section 8: "Exposure controls/personal protection".

### 6.2. Environmental precautions

Avoid release to the environment

#### 6.3. Methods and material for containment and cleaning up

Methods for cleaning up

: Take up liquid spill into absorbent material. Notify authorities if product enters sewers or

public waters.

Other information

: Dispose of materials or solid residues at an authorized site.

#### 6.4. Reference to other sections

For further information refer to section 13.

## **SECTION 7: Handling and storage**

### 7.1. Precautions for safe handling

Precautions for safe handling

: Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Ground/bond container and receiving equipment. Use only non-sparking tools. Take precautionary measures against static discharge. Flammable vapours may accumulate in the container. Use explosion-proof equipment. Wear personal protective equipment. Use only outdoors or in a well-ventilated area. Avoid breathing

dust/fume/gas/mist/vapours/spray.

Hygiene measures : Do not eat, drink or smoke when using this product. Always wash hands after handling the

product.

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

Technical measures

: Ground/bond container and receiving equipment.

Storage conditions

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

#### 7.3. Specific end use(s)

No additional information available

## SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

#### 8.1.1 National occupational exposure and biological limit values

#### 2,6-DIMETHYL-4-HEPTANONE (108-83-8)

#### **Portugal - Occupational Exposure Limits**

Local name Di-isobutilcetona

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2,6-DIMETHYL-4-HEPTANONE (108-83-8)		
OEL TWA [ppm]	25 ppm	
Regulatory reference	Norma Portuguesa NP 1796:2014	
Spain - Occupational Exposure Limits		
Local name	Diisobutilcetona	
VLA-ED (OEL TWA) [1]	148 mg/m³	
VLA-ED (OEL TWA) [2]	25 ppm	
Regulatory reference	Límites de Exposición Profesional para Agentes Químicos en España 2022. INSHT	
United Kingdom - Occupational Exposure Limits		
Local name	2,6-Dimethylheptan-4-one	
WEL TWA (OEL TWA) [1]	148 mg/m³	
WEL TWA (OEL TWA) [2]	25 ppm	
Regulatory reference	EH40/2005 (Fourth edition, 2020). HSE	
USA - ACGIH - Occupational Exposure Limits		
Local name	Diisobutyl ketone	
ACGIH OEL TWA [ppm]	25 ppm	
Remark (ACGIH)	TLV® Basis: URT & eye irr	
Regulatory reference	ACGIH 2022	

### 8.1.2. Recommended monitoring procedures

No additional information available

#### 8.1.3. Air contaminants formed

No additional information available

### 8.1.4. DNEL and PNEC

No additional information available

#### 8.1.5. Control banding

No additional information available

## 8.2. Exposure controls

### 8.2.1. Appropriate engineering controls

#### Appropriate engineering controls:

Ensure good ventilation of the work station.

## 8.2.2. Personal protection equipment

#### Personal protective equipment symbol(s):







## 8.2.2.1. Eye and face protection

#### Eye protection:

Chemical goggles or safety glasses

### 8.2.2.2. Skin protection

## Hand protection:

Protective gloves

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#### 8.2.2.3. Respiratory protection

#### Respiratory protection:

Wear appropriate mask

#### 8.2.2.4. Thermal hazards

No additional information available

#### 8.2.3. Environmental exposure controls

#### **Environmental exposure controls:**

Avoid release to the environment.

## **SECTION 9: Physical and chemical properties**

## 9.1. Information on basic physical and chemical properties

Physical state : Liquid
Appearance : Clear liquid.
Molecular mass : 142.24 g/mol

Colour : Colourless to Light yellow. Odour : sweet, fruity odour. Odour threshold : No data available : No data available рΗ Relative evaporation rate (butylacetate=1) : No data available Melting point : Not applicable Freezing point : -46 °C : 165 – 170 °C Boiling point : 49 °C Flash point Auto-ignition temperature : 345 °C

Decomposition temperature : No data available
Flammability (solid, gas) : Not applicable
Vapour pressure : 1 hPa at 20°C
Relative vapour density at 20 °C : 4.91 (Air = 1.0)
Relative density : No data available
Density : 0.808 g/cm³ at 25°C
Solubility : Water: Immiscible
Ethanol: Miscible

Ethanol: Miscible
Ether: Miscible
No data available

Partition coefficient n-octanol/water (Log Pow) : No data available Viscosity, kinematic : 1.3 mm²/s

Viscosity, dynamic : 1.05 mPa.s at 20°C
Explosive properties : No data available
Oxidising properties : No data available
Lower explosive limit (LEL) : 0.8 vol %
Upper explosive limit (UEL) : 6.2 vol %

#### 9.2. Other information

Refractive index : 1.41 – 1.418 (20°C, 589 nm)

## **SECTION 10: Stability and reactivity**

#### 10.1. Reactivity

Flammable liquid and vapour.

### 10.2. Chemical stability

Stable under normal conditions.

#### 10.3. Possibility of hazardous reactions

No dangerous reactions known under normal conditions of use.

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#### 10.4. Conditions to avoid

Avoid contact with hot surfaces. Heat. No flames, no sparks. Eliminate all sources of ignition.

### 10.5. Incompatible materials

No additional information available

#### 10.6. Hazardous decomposition products

Under normal conditions of storage and use, hazardous decomposition products should not be produced.

## **SECTION 11: Toxicological information**

## 11.1 Information on toxicological effects

Acute toxicity (oral) : Not classified : Not classified Acute toxicity (dermal) Acute toxicity (inhalation) : Not classified Skin corrosion/irritation : Not classified Serious eye damage/irritation : Not classified Respiratory or skin sensitisation : Not classified Germ cell mutagenicity : Not classified Carcinogenicity : Not classified Reproductive toxicity : Not classified

STOT-single exposure : May cause respiratory irritation.

STOT-repeated exposure : Not classified
Aspiration hazard : Not classified

#### **2,6-DIMETHYL-4-HEPTANONE (108-83-8)**

Viscosity, kinematic 1.3 mm<sup>2</sup>/s

## **SECTION 12: Ecological information**

## 12.1. Toxicity

Ecology - general : The product is not considered harmful to aquatic organisms nor to cause long-term adverse

effects in the environment.

: Not classified

Hazardous to the aquatic environment, short-term

(acute)

Hazardous to the aquatic environment, long-term : Not classified

(chronic)

## 12.2. Persistence and degradability

No additional information available

#### 12.3. Bioaccumulative potential

No additional information available

#### 12.4. Mobility in soil

No additional information available

#### 12.5. Results of PBT and vPvB assessment

No additional information available

## 12.6. Other adverse effects

No additional information available

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### **SECTION 13: Disposal considerations**

#### 13.1. Waste treatment methods

Waste treatment methods : Dispose of contents/container in accordance with licensed collector's sorting instructions.

Additional information : Flammable vapours may accumulate in the container.

## **SECTION 14: Transport information**

In accordance with ADR / IMDG / IATA / ADN / RID

### 14.1 UN number

 UN-No. (ADR)
 : UN 1157

 UN-No. (IMDG)
 : UN 1157

 UN-No. (IATA)
 : UN 1157

 UN-No. (ADN)
 : UN 1157

 UN-No. (RID)
 : UN 1157

### 14.2. UN proper shipping name

Proper Shipping Name (ADR) : DIISOBUTYL KETONE
Proper Shipping Name (IMDG) : DIISOBUTYL KETONE
Proper Shipping Name (IATA) : Diisobutyl ketone
Proper Shipping Name (ADN) : DIISOBUTYL KETONE
Proper Shipping Name (RID) : DIISOBUTYL KETONE

Transport document description (ADR) : UN 1157 DIISOBUTYL KETONE, 3, III, (D/E)
Transport document description (IMDG) : UN 1157 DIISOBUTYL KETONE, 3, III (49°C c.c.)

Transport document description (IATA)

: UN 1157 Diisobutyl ketone, 3, III

Transport document description (ADN)

: UN 1157 DIISOBUTYL KETONE, 3, III

Transport document description (RID)

: UN 1157 DIISOBUTYL KETONE, 3, III

### 14.3. Transport hazard class(es)

#### **ADR**

Transport hazard class(es) (ADR) : 3
Danger labels (ADR) : 3



### **IMDG**

Transport hazard class(es) (IMDG) : 3
Danger labels (IMDG) : 3



#### IATA

Transport hazard class(es) (IATA) : 3
Danger labels (IATA) : 3



#### ADN

Transport hazard class(es) (ADN) : 3
Danger labels (ADN) : 3

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RID

Transport hazard class(es) (RID) : 3
Danger labels (RID) : 3



#### 14.4. Packing group

Packing group (ADR) : III
Packing group (IMDG) : III
Packing group (IATA) : III
Packing group (ADN) : III
Packing group (RID) : III

#### 14.5. Environmental hazards

Dangerous for the environment : No Marine pollutant : No

Other information : No supplementary information available

### 14.6. Special precautions for user

#### **Overland transport**

Classification code (ADR) : F1
Limited quantities (ADR) : 5I
Excepted quantities (ADR) : E1

Packing instructions (ADR) : P001, IBC03, LP01, R001

Mixed packing provisions (ADR) : MP19
Portable tank and bulk container instructions (ADR) : T2
Portable tank and bulk container special provisions : TP1

(ADR)

Tank code (ADR) : LGBF
Vehicle for tank carriage : FL
Transport category (ADR) : 3
Special provisions for carriage - Packages (ADR) : V12
Special provisions for carriage - Operation (ADR) : S2
Hazard identification number (Kemler No.) : 30

Orange plates :

30 1157

Tunnel restriction code (ADR) : D/E EAC code : 3Y

#### Transport by sea

: 5 L Limited quantities (IMDG) Excepted quantities (IMDG) : E1 : P001, LP01 Packing instructions (IMDG) IBC packing instructions (IMDG) : IBC03 Tank instructions (IMDG) : T2 Tank special provisions (IMDG) TP1 EmS-No. (Fire) : F-E : S-D EmS-No. (Spillage) Stowage category (IMDG) Α Flash point (IMDG) 49°C c.c.

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Properties and observations (IMDG) : Colourless liquid. Flashpoint: 49°C c.c. Explosive limits: 0.8% to 7.1% Immiscible with

water.

#### Air transport

PCA Excepted quantities (IATA) : E1 PCA Limited quantities (IATA) : Y344 PCA limited quantity max net quantity (IATA) : 10L PCA packing instructions (IATA) : 355 : 60L PCA max net quantity (IATA) : 366 CAO packing instructions (IATA) : 220L CAO max net quantity (IATA) ERG code (IATA) : 3L

#### Inland waterway transport

Classification code (ADN) : F1
Limited quantities (ADN) : 5 L
Excepted quantities (ADN) : E1
Carriage permitted (ADN) : T

Equipment required (ADN) : PP, EX, A
Ventilation (ADN) : VE01
Number of blue cones/lights (ADN) : 0

#### Rail transport

Classification code (RID) : F1
Limited quantities (RID) : 5L
Excepted quantities (RID) : E1

Packing instructions (RID) : P001, IBC03, LP01, R001

Mixed packing provisions (RID) : MP19
Portable tank and bulk container instructions (RID) : T2
Portable tank and bulk container special provisions : TP1

(RID)

Tank codes for RID tanks (RID) : LGBF
Transport category (RID) : 3
Special provisions for carriage – Packages (RID) : W12
Colis express (express parcels) (RID) : CE4
Hazard identification number (RID) : 30

## 14.7. Transport in bulk according to Annex II of Marpol and the IBC Code

Not applicable

### **SECTION 15: Regulatory information**

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

## 15.1.1. EU-Regulations

## **REACH Annex XVII (Restriction List)**

EU restriction list (REACH Annex XVII)	
Reference code	Applicable on
3(a)	2,6-DIMETHYL-4-HEPTANONE
3(b)	2,6-DIMETHYL-4-HEPTANONE
40.	2,6-DIMETHYL-4-HEPTANONE

## **REACH Annex XIV (Authorisation List)**

2,6-DIMETHYL-4-HEPTANONE is not on the REACH Annex XIV List

#### **REACH Candidate List (SVHC)**

2,6-DIMETHYL-4-HEPTANONE is not on the REACH Candidate List

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#### **PIC Regulation (Prior Informed Consent)**

2,6-DIMETHYL-4-HEPTANONE is not subject to Regulation (EU) No 649/2012 of the European Parliament and of the Council of 4 july 2012 concerning the export and import of hazardous chemicals.

#### **POP Regulation (Persistent Organic Pollutants)**

2,6-DIMETHYL-4-HEPTANONE is not subject to Regulation (EU) No 2019/1021 of the European Parliament and of the Council of 20 June 2019 on persistent organic pollutants

#### Ozone Regulation (1005/2009)

2,6-DIMETHYL-4-HEPTANONE is not subject to REGULATION (EU) No 1005/2009 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 16 September 2009 on substances that deplete the ozone layer.

#### **Explosives Precursors Regulation (2019/1148)**

Contains no substance subject to Regulation (EU) 2019/1148 of the European Parliament and of the Council of 20 June 2019 on the marketing and use of explosives precursors.

#### **Drug Precursors Regulation (273/2004)**

Contains no substance(s) listed on the Drug Precursors list (Regulation EC 273/2004 on drug precursors)

#### 15.1.2. National regulations

#### Germany

Employment restrictions : Observe restrictions according Act on the Protection of Working Mothers (MuSchG).

Observe restrictions according Act on the Protection of Young People in Employment

(JArbSchG).

Water hazard class (WGK) : WGK 1, Slightly hazardous to water (Classification according to AwSV; ID No. 591).

Hazardous Incident Ordinance (12. BImSchV) : Is not subject of the Hazardous Incident Ordinance (12. BImSchV)

#### **Netherlands**

SZW-lijst van kankerverwekkende stoffen : The substance is not listed SZW-lijst van mutagene stoffen : The substance is not listed

SZW-lijst van reprotoxische stoffen – Borstvoeding : The substance is not listed SZW-lijst van reprotoxische stoffen – : The substance is not listed

Vruchtbaarheid

SZW-lijst van reprotoxische stoffen – Ontwikkeling : The substance is not listed

#### **Denmark**

Class for fire hazard : Class II-1 Store unit : 5 liter

Classification remarks : R10 <H226;H335>; Emergency management guidelines for the storage of flammable liquids

must be followed

Danish National Regulations : Young people below the age of 18 years are not allowed to use the product

**Switzerland** 

Storage class (LK) : LK 3 - Flammable liquids

## 15.2. Chemical safety assessment

No chemical safety assessment has been carried out

## **SECTION 16: Other information**

Abbreviations and acronyms:	
ADN	European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways
ADR	European Agreement concerning the International Carriage of Dangerous Goods by Road
ATE	Acute Toxicity Estimate
BCF	Bioconcentration factor
BLV	Biological limit value
BOD	Biochemical oxygen demand (BOD)

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Abbreviations and acronyms:		
COD	Chemical oxygen demand (COD)	
DMEL	Derived Minimal Effect level	
DNEL	Derived-No Effect Level	
EC-No.	European Community number	
EC50	Median effective concentration	
EN	European Standard	
IARC	International Agency for Research on Cancer	
IATA	International Air Transport Association	
IMDG	International Maritime Dangerous Goods	
LC50	Median lethal concentration	
LD50	Median lethal dose	
LOAEL	Lowest Observed Adverse Effect Level	
NOAEC	No-Observed Adverse Effect Concentration	
NOAEL	No-Observed Adverse Effect Level	
NOEC	No-Observed Effect Concentration	
OECD	Organisation for Economic Co-operation and Development	
OEL	Occupational Exposure Limit	
PBT	Persistent Bioaccumulative Toxic	
PNEC	Predicted No-Effect Concentration	
RID	Regulations concerning the International Carriage of Dangerous Goods by Rail	
SDS	Safety Data Sheet	
STP	Sewage treatment plant	
ThOD	Theoretical oxygen demand (ThOD)	
TLM	Median Tolerance Limit	
VOC	Volatile Organic Compounds	
CAS-No.	Chemical Abstract Service number	
N.O.S.	Not Otherwise Specified	
vPvB	Very Persistent and Very Bioaccumulative	
ED	Endocrine disrupting properties	

Full text of H- and EUH-statements:	
Flam. Liq. 3	Flammable liquids, Category 3
H226	Flammable liquid and vapour.
H335	May cause respiratory irritation.
STOT SE 3	Specific target organ toxicity – Single exposure, Category 3, Respiratory tract irritation

Safety Data Sheet (SDS), EU

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.