

SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1. Product identifier

Product Description: 2,6-Dimethyl-4-heptanone, remainder mainly 4,6-dimethyl-2-heptanone
 Cat No. : 149440000; 149440010; 149440025; 149440200; 149440250
 Synonyms Diisobutyl ketone
 Index No 606-005-00-X
 CAS No 108-83-8
 Molecular Formula C9 H18 O

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

Recommended Use Laboratory chemicals.
 Uses advised against No Information available

1.3. Details of the supplier of the safety data sheet

Company

UK entity/business name
 Fisher Scientific UK
 Bishop Meadow Road,
 Loughborough, Leicestershire LE11 5RG, United Kingdom

EU entity/business name
 Thermo Fisher Scientific
 Janssen Pharmaceuticaaan 3a, 2440 Geel, Belgium

E-mail address begel.sdsdesk@thermofisher.com

1.4. Emergency telephone number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11
 Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

SECTION 2: HAZARDS IDENTIFICATION

2.1. Classification of the substance or mixture

CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567

Physical hazards

Flammable liquids

Category 3 (H226)

Health hazards

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Specific target organ toxicity - (single exposure)

Category 3 (H335)

Environmental hazards

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

2.2. Label elements



Signal Word

Warning

Hazard Statements

H226 - Flammable liquid and vapor

H335 - May cause respiratory irritation

Precautionary Statements

P304 + P340 - IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking

P261 - Avoid breathing dust/fume/gas/mist/vapors/spray

2.3. Other hazards

Toxicity to Soil Dwelling Organisms

Toxic to terrestrial vertebrates

This product does not contain any known or suspected endocrine disruptors

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.1. Substances

Component	CAS No	EC No	Weight %	CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
Diisobutylketone	108-83-8	EEC No. 203-620-1	>75	Flam. Liq. 3 (H226) STOT SE 3 (H335)
2-Heptanone, 4,6-dimethyl-	19549-80-5	EEC No. 243-148-3	<25	-

Component	Specific concentration limits (SCL's)	M-Factor	Component notes
Diisobutylketone	STOT SE 3 (H335) :: C>=10%	-	-

Full text of Hazard Statements: see section 16

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SECTION 4: FIRST AID MEASURES

4.1. Description of first aid measures

Eye Contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
Skin Contact	Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Get medical attention.
Ingestion	Do NOT induce vomiting. Clean mouth with water. Get medical attention.
Inhalation	Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Get medical attention.
Self-Protection of the First Aider	Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

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

Difficulty in breathing.

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

Notes to Physician Treat symptomatically.

SECTION 5: FIREFIGHTING MEASURES

5.1. Extinguishing media

Suitable Extinguishing Media

Water spray. Carbon dioxide (CO₂). Dry chemical. Chemical foam. Water mist may be used to cool closed containers.

Extinguishing media which must not be used for safety reasons

No information available.

5.2. Special hazards arising from the substance or mixture

Flammable. Vapors may form explosive mixtures with air. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back.

Hazardous Combustion Products

Carbon monoxide (CO), Carbon dioxide (CO₂).

5.3. Advice for firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

SECTION 6: ACCIDENTAL RELEASE MEASURES

6.1. Personal precautions, protective equipment and emergency procedures

Remove all sources of ignition. Take precautionary measures against static discharges.

6.2. Environmental precautions

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See Section 12 for additional Ecological Information.

6.3. Methods and material for containment and cleaning up

Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Prevent product from entering drains. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Do not flush into surface water or sanitary sewer system.

6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

SECTION 7: HANDLING AND STORAGE

7.1. Precautions for safe handling

Avoid contact with skin and eyes. Do not breathe mist/vapors/spray. Use spark-proof tools and explosion-proof equipment. Use only non-sparking tools. Use only in well-ventilated areas. Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharges.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

7.2. Conditions for safe storage, including any incompatibilities

Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Keep away from heat, sparks and flame. Flammables area.

Technical Rules for Hazardous Substances (TRGS) 510 Class 3
Storage Class (LGK) (Germany)

7.3. Specific end use(s)

Use in laboratories

SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1. Control parameters

Exposure limits

List source(s): **UK** - EH40/2005 Work Exposure Limits, Fourth edition. Published 2020. **IRE** - 2021 Code of Practice for the Chemical Agents Regulations, Schedule 1. Published by the Health and Safety Authority

Component	The United Kingdom	European Union	Ireland
Diisobutylketone	STEL: 75 ppm 15 min STEL: 444 mg/m ³ 15 min TWA: 25 ppm 8 hr TWA: 148 mg/m ³ 8 hr		TWA: 25 ppm 8 hr. TWA: 150 mg/m ³ 8 hr. STEL: 75 ppm 15 min STEL: 450 mg/m ³ 15 min

Biological limit values

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

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Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

Workers; See table for values

Component	Acute effects local (Dermal)	Acute effects systemic (Dermal)	Chronic effects local (Dermal)	Chronic effects systemic (Dermal)
Diisobutylketone 108-83-8 (>75)				DNEL = 7.7mg/kg bw/day

Component	Acute effects local (Inhalation)	Acute effects systemic (Inhalation)	Chronic effects local (Inhalation)	Chronic effects systemic (Inhalation)
Diisobutylketone 108-83-8 (>75)				DNEL = 53mg/m ³

Predicted No Effect Concentration (PNEC)

See values below.

Component	Fresh water	Fresh water sediment	Water Intermittent	Microorganisms in sewage treatment	Soil (Agriculture)
Diisobutylketone 108-83-8 (>75)	PNEC = 0.03mg/L	PNEC = 0.46mg/kg sediment dw	PNEC = 0.3mg/L	PNEC = 2.55mg/L	PNEC = 0.0746mg/kg soil dw

Component	Marine water	Marine water sediment	Marine water intermittent	Food chain	Air
Diisobutylketone 108-83-8 (>75)	PNEC = 0.003mg/L	PNEC = 0.046mg/kg sediment dw			

8.2. Exposure controls

Engineering Measures

Ensure adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting equipment. Ensure that eyewash stations and safety showers are close to the workstation location.

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

Personal protective equipment

Eye Protection Goggles (European standard - EN 166)

Hand Protection Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	See manufacturers recommendations	-	EN 374	(minimum requirement)
Neoprene				
Natural rubber				
PVC				

Skin and body protection Wear appropriate protective gloves and clothing to prevent skin exposure.

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Respiratory Protection When workers are facing concentrations above the exposure limit they must use

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appropriate certified respirators.

To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

Large scale/emergency use

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

Recommended Filter type: Organic gases and vapours filter Type A Brown conforming to EN14387

Small scale/Laboratory use

Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141

When RPE is used a face piece Fit Test should be conducted

Environmental exposure controls No information available.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Physical State	Liquid	
Appearance	Light yellow	
Odor	Mint-like	
Odor Threshold	No data available	
Melting Point/Range	-46 °C / -50.8 °F	
Softening Point	No data available	
Boiling Point/Range	169 °C / 336.2 °F	@ 760 mmHg
Flammability (liquid)	Flammable	On basis of test data
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	Lower 0.8 Vol% Upper 6.2 Vol%	
Flash Point	49 °C / 120.2 °F	Method - No information available
Autoignition Temperature	345 °C / 653 °F	
Decomposition Temperature	No data available	
pH	No information available	
Viscosity	1.05 mPa s at 20 °C	
Water Solubility	0,5 g/l	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Component	log Pow	
Diisobutylketone	3.71	
Vapor Pressure	1 hPa @ 20 °C	
Density / Specific Gravity	0.809	
Bulk Density	Not applicable	Liquid
Vapor Density	4.9	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	

9.2. Other information

Molecular Formula	C9 H18 O
Molecular Weight	142.24
Explosive Properties	explosive air/vapour mixtures possible

SECTION 10: STABILITY AND REACTIVITY

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10.1. Reactivity

None known, based on information available

10.2. Chemical stability

Stable under recommended storage conditions.

10.3. Possibility of hazardous reactions

Hazardous Polymerization Hazardous Reactions

Hazardous polymerization does not occur.
No information available.

10.4. Conditions to avoid

Keep away from open flames, hot surfaces and sources of ignition. Incompatible products.

10.5. Incompatible materials

Strong oxidizing agents. Strong bases. Strong reducing agents.

10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO₂).

SECTION 11: TOXICOLOGICAL INFORMATION

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Product Information

(a) acute toxicity;

Oral

Based on available data, the classification criteria are not met

Dermal

Based on available data, the classification criteria are not met

Inhalation

Based on available data, the classification criteria are not met

Toxicology data for the components

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Diisobutylketone	LD50 = 5750 mg/kg (Rat)	LD50 > 2000 mg/kg (Rat)	LC50 > 2300 ppm (Rat) 4 h

(b) skin corrosion/irritation;

No data available

(c) serious eye damage/irritation;

No data available

(d) respiratory or skin sensitization;

Respiratory

No data available

Skin

No data available

(e) germ cell mutagenicity;

No data available

(f) carcinogenicity;

No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity;

No data available

(h) STOT-single exposure;

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Results / Target organs Respiratory system.

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; No data available

Other Adverse Effects

Symptoms / effects, both acute and delayed No information available.

11.2. Information on other hazards

Endocrine Disrupting Properties Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

SECTION 12: ECOLOGICAL INFORMATION

12.1. Toxicity

Ecotoxicity effects

Do not flush into surface water or sanitary sewer system. Do not allow material to contaminate ground water system. Do not empty into drains.

Component	Freshwater Fish	Water Flea	Freshwater Algae
Diisobutylketone	LC50: 140 mg/L, 96h semi-static (Oncorhynchus mykiss)	EC50: 37,2 mg/L/48H	EC50: 100 mg/L, 96h (Pseudokirchneriella subcapitata)

12.2. Persistence and degradability

Persistence

Readily biodegradable
Insoluble in water, May persist, based on information available.

12.3. Bioaccumulative potential

May have some potential to bioaccumulate

Bioconcentration factor (BCF)

130

Component	log Pow	Bioconcentration factor (BCF)
Diisobutylketone	3.71	No data available

12.4. Mobility in soil

Spillage unlikely to penetrate soil The product is insoluble and floats on water The product evaporates slowly Is not likely mobile in the environment due its low water solubility.
Spillage unlikely to penetrate soil

12.5. Results of PBT and vPvB assessment

No data available for assessment.

12.6. Endocrine disrupting properties

Endocrine Disruptor Information

This product does not contain any known or suspected endocrine disruptors

12.7. Other adverse effects

Persistent Organic Pollutant

This product does not contain any known or suspected substance

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Ozone Depletion Potential This product does not contain any known or suspected substance

SECTION 13: DISPOSAL CONSIDERATIONS

13.1. Waste treatment methods

Waste from Residues/Unused Products Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

Contaminated Packaging Dispose of this container to hazardous or special waste collection point. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and empty container away from heat and sources of ignition.

European Waste Catalogue (EWC) According to the European Waste Catalog, Waste Codes are not product specific, but application specific.

Other Information Waste codes should be assigned by the user based on the application for which the product was used. Do not flush to sewer. Can be landfilled or incinerated, when in compliance with local regulations.

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

14.1. UN number UN1157
14.2. UN proper shipping name DIISOBUTYL KETONE
14.3. Transport hazard class(es) 3
14.4. Packing group III

ADR

14.1. UN number UN1157
14.2. UN proper shipping name DIISOBUTYL KETONE
14.3. Transport hazard class(es) 3
14.4. Packing group III

IATA

14.1. UN number UN1157
14.2. UN proper shipping name DIISOBUTYL KETONE
14.3. Transport hazard class(es) 3
14.4. Packing group III

14.5. Environmental hazards No hazards identified

14.6. Special precautions for user No special precautions required.

14.7. Maritime transport in bulk according to IMO instruments Not applicable, packaged goods

SECTION 15: REGULATORY INFORMATION

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

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International Inventories

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
Diisobutylketone	108-83-8	203-620-1	-	-	X	X	KE-10907	X	X
2-Heptanone, 4,6-dimethyl-	19549-80-5	243-148-3	-	-	X	X	KE-11439	X	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Diisobutylketone	108-83-8	X	ACTIVE	X	-	X	X	X
2-Heptanone, 4,6-dimethyl-	19549-80-5	X	ACTIVE	X	-	-	X	X

Legend: X - Listed '-' - Not Listed

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

Authorisation/Restrictions according to EU REACH

Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Diisobutylketone	108-83-8	-	-	-
2-Heptanone, 4,6-dimethyl-	19549-80-5	-	-	-

Seveso III Directive (2012/18/EC)

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements
Diisobutylketone	108-83-8	Not applicable	Not applicable
2-Heptanone, 4,6-dimethyl-	19549-80-5	Not applicable	Not applicable

Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

National Regulations

UK - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

WGK Classification

Water endangering class = 1 (self classification)

Component	Germany - Water Classification (AwSV)	Germany - TA-Luft Class
Diisobutylketone	WGK1	

Component	France - INRS (Tables of occupational diseases)
Diisobutylketone	Tableaux des maladies professionnelles (TMP) - RG 84

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15.2. Chemical safety assessment

Chemical Safety Assessment/Reports (CSA/CSR) are not required for mixtures

SECTION 16: OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3

H226 - Flammable liquid and vapor

H335 - May cause respiratory irritation

Legend

CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit

ACGIH - American Conference of Governmental Industrial Hygienists

DNEL - Derived No Effect Level

RPE - Respiratory Protective Equipment

LC50 - Lethal Concentration 50%

NOEC - No Observed Effect Concentration

PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer Predicted No Effect Concentration (PNEC)

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

VOC - (Volatile Organic Compound)

Classification and procedure used to derive the classification for mixtures according to Regulation (EC) 1272/2008 [CLP]:

Physical hazards On basis of test data

Health Hazards Calculation method

Environmental hazards Calculation method

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Creation Date 09-May-2012

Revision Date 21-Sep-2023

Revision Summary Not applicable.

This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.

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Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of Safety Data Sheet