# SAFETY DATA SHEET (SDS)

in accordance with Regulation (EC) No 1907/2006 (REACH), Annex II — Regulation (EU) 2020/878

Date: 05.11.2026 | Version: 10 | EN

## 2,6-dimethylheptan-4-one

*2,6-dimethylheptan-4-one*

**CAS 108-83-8**

$C_9H_{18}O$ | EC 203-620-1

| MOLAR MASS | LOGP |
|---|---|
| 142.24 | 2.5 |

### HAZARD CLASSIFICATION (GHS / CLP)



**Warning**

H226 | H335

*Hazard class scope limited to the harmonised classification (CLP Annex VI); classes outside the harmonised entry may require supplier self-classification (CLP Art. 4(3)) — verify with the supplier safety data sheet.*

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

| | |
|---|---|
| **1.1 Substance name** | 2,6-dimethylheptan-4-one |
| **1.1 IUPAC name** | 2,6-dimethylheptan-4-one |
| **1.1 CAS number** | 108-83-8 |
| **1.1 EC number** | 203-620-1 |
| **1.1 PubChem CID** | 7958 |
| **1.1 InChIKey** | PTTPXKJBFFKCEK-UHFFFAOYSA-N |
| **1.1 SMILES** | CC(C)CC(=O)CC(C)C |
| **1.1 Molecular formula** | $C_9H_{18}O$ [7] |
| **1.1 Molar mass** | 142.24 g/mol [7] |
| **1.1 Exact mass** | 142.1358 Da [7] |

### 1.2 Uses

For laboratory and research purposes. Not for use in the production of food, medicines or cosmetics without appropriate authorisation.

### 1.3 Details of the supplier

| | |
|---|---|
| REFERENCE COPY — NO SUPPLIER DETAILS — NOT FOR DISTRIBUTION | Supplier details are not included in this reference copy. The supplier placing the substance on the market must complete this section and remains responsible for the sheet under REACH. MolGod.org prepares documentation and is not the supplier of this substance. |

### 1.4 Emergency telephone number

| | |
|---|---|
| **Emergency telephone** | 112 (EU-wide emergency number) |

Contact the poison centre designated in the country of placing on the market (CLP Art. 45).

## 2. Hazards identification

**GHS:**



**PPE:**



**Prohibitions:**



**Warning**

### Hazard statements (H) [3][4][10]

| | |
|---|---|
| **H226** | Flammable liquid and vapour |
| **H335** | May cause respiratory irritation |

### Precautionary statements (P) [3][4][10]

| | |
|---|---|
| **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 |
| **P261** | Avoid breathing dust/fume/gas/mist/vapours/spray |
| **P271** | Use only outdoors or in a well-ventilated area |
| **P280** | Wear protective gloves/protective clothing/eye protection/face protection |
| **P303+P361+P353** | IF ON SKIN (or hair): Take off immediately all contaminated clothing; Rinse skin with water or shower |
| **P304+P340** | IF INHALED: Remove person to fresh air and keep comfortable for breathing |
| **P312** | Call a POISON CENTER or doctor/physician if you feel unwell |
| **P370+P378** | In case of fire: Use appropriate media to extinguish |
| **P403+P235** | Store in a well-ventilated place: Keep cool |
| **P403+P233** | Store in a well-ventilated place: Keep container tightly closed |
| **P405** | Store locked up |
| **P501** | Dispose of contents/container to an approved waste collection point |

**Hazard class scope limited to the harmonised classification (CLP Annex VI); classes outside the harmonised entry may require supplier self-classification (CLP Art. 4(3)) — verify with the supplier safety data sheet.**

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## 3. Composition/information on ingredients

| | |
|---|---|
| **Substance type** | pure substance |
| **CAS Number** | 108-83-8 |
| **EC number** | 203-620-1 |
| **Molecular formula** | $C_9H_{18}O$ |
| **Concentration** | ≥99% (typical reagent-grade purity — to be confirmed by the supplier's specification) |
| **Clp index no** | 606-005-00-X |
| **Specific concentration limits / M-factor (CLP Annex VI Table 3)** | SCL: H335: C ≥ 10 % [3] |

## 4. First aid measures



### Inhalation

Move the affected person to fresh air. Keep at rest. If not breathing: artificial respiration (qualified personnel only). [1][2][12]

### Skin contact

Remove contaminated clothing. Rinse skin with soap and water (min. 15 minutes). [1][2][12]

### Eye contact

Rinse eyes with running water (min. 15 minutes). Remove contact lenses if possible. If irritation persists — consult an ophthalmologist. [1][2][12]

### Ingestion

Do NOT induce vomiting (unless directed by a physician). Rinse mouth with water. Never give anything by mouth to an unconscious person. Emergency number: 112 (EU-wide). Contact the poison centre designated in your country (CLP Art. 45). [1][2][12]

### Symptoms and effects

cough, shortness of breath, headache, dizziness. [3][10]

### Notes for physician

Requires verification

**Emergency numbers: Emergency: 112 (EU-wide). Poison centre: as designated in the country of placing on the market (CLP Art. 45).**

## 5. Firefighting measures

| | |
|---|---|
| **Suitable extinguishing media** | Alcohol-resistant foam, carbon dioxide ($CO_2$), dry chemical powder, water spray/mist. [1][2][12] |
| **Unsuitable extinguishing media** | Full/compact water jet (splashes and spreads the burning liquid, which floats on water). [1][2][12] |
| **Specific hazards** | Thermal decomposition products: CO, CO2. [13] |
| **Advice for firefighters** | Use self-contained breathing apparatus (SCBA). Full protective suit. [1][2][12] |
| **Flash Point** | 48.9°C [7] |
| **Auto-ignition temperature** | 396.1°C [7] |

## 6. Accidental release measures

| | |
|---|---|
| **Personal precautions** | Use personal protective equipment (see Section 8). Avoid breathing vapours. [1][2][12] |
| **Environmental precautions** | Prevent entry into sewers, groundwater and surface water. [1][2][12] |
| **Methods for containment and cleaning up** | Contain the spill with a barrier. Absorb with inert material (sand, vermiculite, diatomaceous earth). Collect into sealed, labelled containers. Do not release into drains. Remove ignition sources; use non-sparking tools. [1][2][12] |
| **Related sections** | 8; 13 |

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## 7. Handling and storage

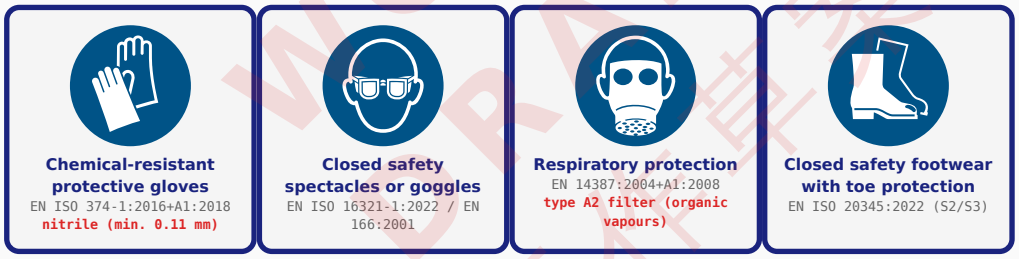
| | |
|---|---|
| **Precautions** | Work in a fume hood or with adequate ventilation. No eating, drinking or smoking in the work area. [1][2][12] |
| **Storage temperature** | Store at room temperature (15-25°C) or as indicated on the label. [1][2][12] |
| **Humidity** | Store in a dry place (<60% RH). [1][2][12] |
| **Light** | Protect from direct sunlight. [1][2][12] |
| **Incompatible materials** | Strong oxidizers, Ignition sources, open flames. [13] |

## 8. Exposure controls/personal protection

### 8.1 Control parameters

| | |
|---|---|
| **OEL — NDS (Poland)** | No NDS (OEL) value in the available working list — verify in the current MRPiPS regulation before use; do not assume the absence of a limit value. |
| **OEL (EU)** | The EU OEL value has not been verified against the available dataset — check the IOELV/BOELV directives; do not assume the absence of a value. |
| **DNEL** | No data available. |
| **PNEC** | No data available. |

### 8.2 Personal protective equipment (PPE) [5][6][14]



**Chemical-resistant protective gloves**
EN ISO 374-1:2016+A1:2018
nitrile (min. 0.11 mm)

**Closed safety spectacles or goggles**
EN ISO 16321-1:2022 / EN 166:2001

**Respiratory protection**
EN 14387:2004+A1:2008
type A2 filter (organic vapours)

**Closed safety footwear with toe protection**
EN ISO 20345:2022 (S2/S3)

## 9. Physical and chemical properties

| Property (item 9.1) | Value | Source |
|---|---|---|
| **Physical state** | Liquid | |
| **Colour** | No data available. | |
| **Odour** | Peppermint odor [7] | |
| **pH (1% aqueous solution)** | No data available. | |
| **Melting point** | -41.5673°C [8] [7] | |
| **Boiling point** | 168.3904°C [8] [7] | |
| **Flash point** | 48.9°C (experimental data) [7] | |
| **Flammability** | Flam. Liq. 3 (H226) [3][10] | |
| **Lower and upper explosion limit** | No data available. | |
| **Density (20°C)** | 0.8075 g/cm³ [7] | |
| **Vapour pressure** | 0.22 kPa (1.65 mmHg, 25°C) (experimental data) [7] | |
| **Relative vapour density** | 4.91 [17] | |
| **Dynamic viscosity** | 0.896 mPa·s [7] | |

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| Property (item 9.1) | Value | Source |
|---|---|---|
| **Kinematic viscosity** | No data available. | |
| **Refractive index nD²⁰** | 1.41 (experimental data) [7] | |
| **Auto-ignition temperature** | 396.1°C (experimental data) [7] | |
| **Decomposition temperature** | Not applicable | |
| **Water solubility** | No data available. | |
| **Particle characteristics** | Not applicable (REACH 9.1(r)) | |
| **Partition coefficient n-octanol/water (log value)** | 2.5 [9] | |
| **Molar mass** | 142.24 g/mol [7] | |
| **Molecular formula** | $C_9H_{18}O$ [7] | |
| **Lipinski rule (RO5)** | **PASS** | |

Where a property above reads "No data available", no measured value was found in the public sources consulted for this substance. The property has not been determined by MolGod.org and no value is inferred. "Not applicable" means the property has no meaning for this substance in the form supplied.

## 10. Stability and reactivity

| | |
|---|---|
| **Reactivity** | Stable under normal storage and handling conditions. |
| **Chemical stability** | Thermally stable under recommended conditions. |
| **Hazardous reactions** | No hazardous reactions known under normal conditions. |
| **Conditions to avoid** | High temperatures, direct sunlight, moisture. |
| **Incompatible materials** | Strong oxidizers, Ignition sources, open flames. |
| **Decomposition products** | Thermal decomposition products: CO, CO2. |

## 11. Toxicological information

| | |
|---|---|
| **LD50 (oral)** | No data available. |
| **LD50 (dermal)** | LD50 >2000 mg/kg (rat) [7] |
| **LC50 (inhalation)** | No data available. |
| **Skin irritation** | Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10] |
| **Eye irritation** | Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10] |
| **Sensitisation** | Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10] |
| **Mutagenicity** | Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10] |
| **Carcinogenicity** | Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10] |
| **IARC classification (carcinogenicity)** | No individual IARC monograph for this CAS — this is not confirmation of the absence of carcinogenicity (cf. CLP/GHS classification in section 2). |
| **Reproductive toxicity** | Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10] |
| **STOT — single exposure** | Category 3 (H335): May cause respiratory irritation. [3][10] |
| **STOT — repeated exposure** | Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10] |

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| | |
|---|---|
| **Aspiration hazard** | Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10] |

## 12. Ecological information

| | |
|---|---|
| **Aquatic toxicity** | No data available. |
| **Persistence / biodegradability** | No data available. |
| **Bioaccumulative potential** | log Kow = 2.5 [9]. Low bioaccumulation potential (log Kow < 4.5 — PBT/vPvB screening criterion per ECHA Guidance R.11). [15][16] |
| **Mobility in soil** | No data available. |
| **PBT/vPvB assessment** | Insufficient data to assess PBT/vPvB. |
| **Endocrine disrupting properties** | No information. |

## 13. Disposal considerations

| | |
|---|---|
| **Disposal method** | Hand over for disposal to licensed contractors in accordance with national and local regulations. Do not discharge into sewers. |
| **Waste code (EWC)** | 16 05 06* — Laboratory and analytical chemicals (e.g. chemical reagents) containing hazardous substances. Verification of the EWC code required. [11] |
| **Packaging** | Cleaned packaging may be recycled. Contaminated packaging must be treated as hazardous waste. |

## 14. Transport information




Class 3 — Flammable liquids

| | |
|---|---|
| **UN number** | UN 1157 [7] |
| **Transport hazard class** | Suggested from GHS classification — VERIFICATION REQUIRED. |
| **Environmental hazard** | Not classified as environmentally hazardous for transport (no H400/H410/H411 in CLP Annex VI; no marine pollutant mark required) [3] |
| **Special precautions** | Handle as dangerous goods according to the assigned class (ADR/IMDG/IATA); apply the precautions appropriate to that class. |
| **CN/HS code** | CN/HS code: verification required in the Eurostat Combined Nomenclature. |
| **Notes** | UN number per the indicated source. Verify the transport class and packing group in ADR Table A / UN Model Regulations before shipment. [7] |

## 15. Regulatory information

| | |
|---|---|
| **SVHC status** | SVHC status not verified against the available dataset — check the current ECHA Candidate List; do not assume absence. [1] |
| **REACH Annex XIV** | Not verified against the ECHA Authorisation List — check REACH Annex XIV. [1] |
| **REACH Annex XVII** | Not confirmed in the available Annex XVII dataset — verify against the current ECHA list before placing on the market; do not assume absence of restriction. [1] |

## 16. Other information

Legal status of classification: harmonised under CLP Annex VI — Reg. (EC) No 1272/2008 (as at the date of issue).Entries with an entry-into-force date after 05.11.2026 were omitted as future (not yet applicable).

**Data aggregated automatically from public reference databases (PubChem, ECHA, NIST and others).**

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## Scientific citations (10)


V. Svoboda, V. Kubeš, P. Basařová. *Enthalpies of vaporization and cohesive energies of hexan-2-one, 2-methylpentan-4-one, 2,2-dimethylbutan-3-one, 2,6-dimethylheptan-4-one, and cyclohexanone*. The Journal of Chemical Thermodynamics (1992). DOI: 10.1016/s0021-9614(05)80074-6

Ch. Wohlfarth. *Dielectric constant of the mixture (1) chlorobenzene; (2) 2,6-dimethylheptan-4-one*. Landolt-Börnstein - Group IV Physical Chemistry (2008). DOI: 10.1007/978-3-540-75506-7_917

Ch. Wohlfarth. *Dielectric constant of the mixture (1) toluene; (2) 2,6-dimethylheptan-4-one*. Landolt-Börnstein - Group IV Physical Chemistry (2008). DOI: 10.1007/978-3-540-75506-7_1010

Ch. Wohlfarth. *Dielectric constant of the mixture (1) butanoic acid; (2) 2,6-dimethylheptan-4-one*. Landolt-Börnstein - Group IV Physical Chemistry (2008). DOI: 10.1007/978-3-540-75506-7_765

Ch. Wohlfarth. *Dielectric constant of the mixture (1) propanoic acid; (2) 2,6-dimethylheptan-4-one*. Landolt-Börnstein - Group IV Physical Chemistry (2008). DOI: 10.1007/978-3-540-75506-7_619


## Full text of H statements

| | |
|---|---|
| **H226** | Flammable liquid and vapour |
| **H335** | May cause respiratory irritation |

## Full text of P statements

| | |
|---|---|
| **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 |
| **P261** | Avoid breathing dust/fume/gas/mist/vapours/spray |
| **P271** | Use only outdoors or in a well-ventilated area |
| **P280** | Wear protective gloves/protective clothing/eye protection/face protection |
| **P303+P361+P353** | IF ON SKIN (or hair): Take off immediately all contaminated clothing; Rinse skin with water or shower |
| **P304+P340** | IF INHALED: Remove person to fresh air and keep comfortable for breathing |
| **P312** | Call a POISON CENTER or doctor/physician if you feel unwell |
| **P370+P378** | In case of fire: Use appropriate media to extinguish |
| **P403+P235** | Store in a well-ventilated place: Keep cool |
| **P403+P233** | Store in a well-ventilated place: Keep container tightly closed |
| **P405** | Store locked up |
| **P501** | Dispose of contents/container to an approved waste collection point |

## Abbreviations

| | |
|---|---|
| **ADR** | European Agreement concerning the International Carriage of Dangerous Goods by Road |
| **ATE** | Acute Toxicity Estimate |
| **CAS** | Chemical Abstracts Service |
| **CLP** | Classification, Labelling and Packaging (Reg. (EC) 1272/2008) |
| **CMR** | Carcinogenic, Mutagenic, toxic to Reproduction |
| **DNEL** | Derived No-Effect Level |
| **EC** | European Community number |
| **EPI** | Personal protective equipment |
| **GHS** | Globally Harmonized System |
| **IATA** | International Air Transport Association |
| **IMDG** | International Maritime Dangerous Goods Code |
| **SDS** | Safety Data Sheet |
| **LC50** | Lethal Concentration, 50% |
| **LD50** | Lethal Dose, 50% |
| **NDS** | Maximum admissible concentration (workplace, PL) |

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| | |
|---|---|
| **NDSCh** | Short-term exposure limit (PL) |
| **OEL** | Occupational Exposure Limit |
| **PBT** | Persistent, Bioaccumulative and Toxic |
| **PNEC** | Predicted No-Effect Concentration |
| **REACH** | Registration, Evaluation, Authorisation and Restriction of Chemicals (Reg. (EC) 1907/2006) |
| **STOT** | Specific Target Organ Toxicity |
| **SVHC** | Substance of Very High Concern |
| **TPSA** | Topological Polar Surface Area |
| **vPvB** | very Persistent and very Bioaccumulative |

## Version history

| | |
|---|---|
| **v10 (05.11.2026)** | Based on ECHA harmonised classification (Annex VI to CLP, ATP 23). |

## References


[1] EP and Council. Reg.(EC) No 1907/2006 (REACH). Art.31, Annex II. OJ EU L 396/2006. URL: https://eur-lex.europa.eu/eli/reg/2006/1907/oj Accessed: 2026-11-05.

[2] European Commission. Reg.(EU) 2020/878 — amending Annex II REACH. OJ EU L 203/2020. From 01.01.2023. URL: https://eur-lex.europa.eu/eli/reg/2020/878/oj Accessed: 2026-11-05.

[3] EP and Council. Reg.(EC) 1272/2008 (CLP) + ATP 23. OJ EU L 353/2008. (2026-07-07) URL: https://eur-lex.europa.eu/eli/reg/2008/1272/oj Accessed: 2026-11-05.

[4] United Nations. GHS Rev.9. ST/SG/AC.10/30/Rev.9. New York and Geneva: United Nations, 2021. URL: https://unece.org/transport/dangerous-goods/ghs-rev9-2021 Accessed: 2026-11-05.

[5] ISO. ISO 7010:2019 — Graphical symbols. Safety signs. URL: https://www.iso.org/standard/72424.html Accessed: 2026-11-05.

[6] ISO. ISO 3864-1:2011 — Safety colours and safety signs. URL: https://www.iso.org/standard/51021.html Accessed: 2026-11-05.

[7] PubChem. National Center for Biotechnology Information (NIH/NLM), chemical compound database. URL: https://pubchem.ncbi.nlm.nih.gov/compound/7958

[8] NIST. Chemistry WebBook, SRD 69. National Institute of Standards and Technology. URL: https://webbook.nist.gov/cgi/cbook.cgi?ID=108-83-8

[9] Rumble, J.R., ed. CRC Handbook of Chemistry and Physics. 105th ed. Boca Raton: CRC Press, 2024. URL: https://hbcp.chemnetbase.com

[10] ECHA. European Chemicals Agency — harmonised classification inventory (CLP Annex VI). URL: https://echa.europa.eu

[11] European Commission. Decision 2000/532/EC establishing a list of wastes (European Waste Catalogue). OJ EU L 226/3. URL: https://eur-lex.europa.eu/eli/dec/2000/532/oj

[12] European Chemicals Agency (ECHA). Guidance on the Compilation of Safety Data Sheets. Version 4.0. Helsinki: European Chemicals Agency, 2020. URL: https://echa.europa.eu/documents/10162/2324906/sds_en.pdf

[13] Urben, P.G., ed. Bretherick's Handbook of Reactive Chemical Hazards. 8th ed. Oxford: Academic Press.

[14] CEN. Personal protective equipment standards (EN ISO 374-1, EN 166, EN 149, EN 14387, EN ISO 20345). Brussels: European Committee for Standardization.

[15] ECHA. Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.11: PBT/vPvB Assessment. Helsinki: European Chemicals Agency. URL: https://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment

[16] European Parliament and Council. Regulation (EC) No 1907/2006 (REACH), Annex XIII — Criteria for the identification of PBT and vPvB substances. OJ EU L 396/2006 (consolidated). URL: https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:02006R1907-20140410

[17] MOL-GOD. Value obtained by calculation from the molecular formula/molecular weight (the specific quantity and its formula are indicated at the respective field). Calculated value, not an experimental measurement. URL: https://www.nist.gov/pml/atomic-weights-and-isotopic-compositions-relative-atomic-masses

[18] MRiPS Regulation of 12.06.2018 — NDS/NDN. Journal of Laws 2024 item 1017. URL: https://isap.sejm.gov.pl/isap.nsf/DocDetails.xsp?id=WDU20240001017 Accessed: 2026-11-05.


## External links

NIST: https://webbook.nist.gov/cgi/cbook.cgi?ID=108-83-8

ChEMBL: https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL3182186

**NFPA 704** (supplementary information — NFPA/USA system; not a required element of an EU safety data sheet under REACH Annex II)





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