SAFETY DATA SHEET (SDS)

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

Date: 04.11.2026 | Version: 10 | EN

Methyl hexanoate

methyl hexanoate

CAS 106-70-7

$C_7H_{14}O_2$ | EC 203-425-1

MOLAR MASS	LOGP
130.18	2.5

HAZARD CLASSIFICATION (GHS / CLP)



Warning

H226

Non-harmonised classification (no entry in Annex VI to CLP) — assigned from aggregated ECHA C&L notifications; the H-statements require verification against the official source (ECHA C&L / manufacturer's data sheet).

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

1.1 Substance name	Methyl hexanoate
1.1 IUPAC name	methyl hexanoate
1.1 CAS number	106-70-7
1.1 EC number	203-425-1
1.1 PubChem CID	7824
1.1 InChIKey	NUKZAGXMHTUAFE-UHFFFAOYSA-N
1.1 SMILES	CCCCCC(=O)OC
1.1 Molecular formula	$C_7H_{14}O_2$ [7]
1.1 Molar mass	130.18 g/mol [7]
1.1 Exact mass	130.0994 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]

H226	Flammable liquid and vapour

Precautionary statements (P) [3][4]

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
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
P370+P378	In case of fire: Use appropriate media to extinguish
P403+P235	Store in a well-ventilated place: Keep cool
P501	Dispose of contents/container to an approved waste collection point

Non-harmonised classification (no entry in Annex VI to CLP) — assigned from aggregated ECHA C&L notifications; the H-statements require verification against the official source (ECHA C&L / manufacturer's data sheet).

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3. Composition/information on ingredients

Substance type	pure substance
CAS Number	106-70-7
EC number	203-425-1
Molecular formula	$C_7H_{14}O_2$
Concentration	≥99% (typical reagent-grade purity — to be confirmed by the supplier's specification)

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][11]

Skin contact

Remove contaminated clothing. Rinse skin with soap and water (min. 15 minutes). [1][2][11]

Eye contact

Rinse eyes with running water (min. 15 minutes). Remove contact lenses if possible. If irritation persists — consult an ophthalmologist. [1][2][11]

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][11]

Symptoms and effects

No specific symptoms described in the literature. [3]

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][11]
Unsuitable extinguishing media	Full/compact water jet (splashes and spreads the burning liquid, which floats on water). [1][2][11]
Specific hazards	Thermal decomposition products: CO, CO2. [12]
Advice for firefighters	Use self-contained breathing apparatus (SCBA). Full protective suit. [1][2][11]
Flash Point	72.8°C [7]

6. Accidental release measures

Personal precautions	Use personal protective equipment (see Section 8). Avoid breathing vapours. [1][2][11]
Environmental precautions	Prevent entry into sewers, groundwater and surface water. [1][2][11]
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][11]
Related sections	8; 13

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][11]

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Storage temperature	Store at room temperature (15-25°C) or as indicated on the label. [1][2][11]
Humidity	Store in a dry place (<60% RH). [1][2][11]
Light	Protect from direct sunlight. [1][2][11]
Incompatible materials	Strong oxidizers, Ignition sources, open flames. [12]

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][13]



9. Physical and chemical properties

Property (item 9.1)	Value	Source
Physical state	Liquid	
Colour	No data available.	
Odour	No data available.	
pH (1% aqueous solution)	No data available.	
Melting point	-70.0577°C [8] [7]	
Boiling point	149.2788°C [8] [7]	
Flash point	72.8°C (experimental data) [7]	
Flammability	Flam. Liq. 3 (H226) [3]	
Lower and upper explosion limit	No data available.	
Density (20°C)	0.8848 g/cm³ [7]	
Vapour pressure	0.667 kPa (5 mmHg, 30°C) (experimental data) [7]	
Relative vapour density	4.49 [16]	
Kinematic viscosity	No data available.	
Refractive index nD²⁰	1.402 (experimental data) [7]	
Auto-ignition temperature	No data available.	
Decomposition temperature	Not applicable	

Property (item 9.1)	Value	Source
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	130.18 g/mol [7]	
Molecular formula	$C_7H_{14}O_2$ [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)	No data available.
LC50 (inhalation)	No data available.
Skin irritation	No data available.
Eye irritation	No data available.
Sensitisation	No data available.
Mutagenicity	No data available.
Carcinogenicity	No data available.
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	No data available.
STOT — single exposure	No data available.
STOT — repeated exposure	No data available.
Aspiration hazard	No data available.

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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). [14][15]
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. [10]
Packaging	Cleaned packaging may be recycled. Contaminated packaging must be treated as hazardous waste.

14. Transport information



Class 3 — Flammable liquids

UN number	UN 1993 [7]
Transport hazard class	Suggested from GHS classification — VERIFICATION REQUIRED.
Environmental hazard	Environmental hazard for transport: not verified. Non-harmonised classification (outside CLP Annex VI) — verify aquatic toxicity (Section 12) and do NOT assume marine pollutant marking is not required; confirm per ADR 2.2.9 / IMDG before shipping.
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: supplier self-classification under Art. 4(3) CLP — no harmonised entry in Annex VI.Entries with an entry-into-force date after 04.11.2026 were omitted as future (not yet applicable).

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

Scientific citations (8)

Api AM, Belsito D, Botelho D et al.. *RIFM fragrance ingredient safety assessment, methyl hexanoate, CAS Registry Number 106-70-7.*. Food and chemical toxicology : an international journal published for the British Industrial Biological Research Association (2021). DOI: 10.1016/j.fct.2021.112572

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Jiang Y, Liu G, Zhang W et al.. *Biosynthesis and emission of methyl hexanoate, the major constituent of floral scent of a night-blooming water lily Victoriacruziana.*. Phytochemistry (2021). DOI: 10.1016/j.phytochem.2021.112899

Dang NN, Pham HN, Kleiner I et al.. *Methyl Internal Rotation in Fruit Esters: Chain-Length Effect Observed in the Microwave Spectrum of Methyl Hexanoate.*. Molecules (Basel, Switzerland) (2022). DOI: 10.3390/molecules27092639

Ensari Y, de Almeida Santos G, Ruff AJ et al.. *Engineered P450 BM3 and cpADH5 coupled cascade reaction for β-oxo fatty acid methyl ester production in whole cells.*. Enzyme and microbial technology (2020). DOI: 10.1016/j.enzmictec.2020.109555

Supriyadi, Suzuki M, Wu S et al.. *Biogenesis of volatile methyl esters in snake fruit (Salacca edulis, Reinw) cv. Pondoh.*. Bioscience, biotechnology, and biochemistry (2003). DOI: 10.1271/bbb.67.1267

Full text of H statements

H226	Flammable liquid and vapour

Full text of P statements

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

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Version history

v10 (04.11.2026)	Based on supplier self-classification (ECHA C&L notifications; no harmonised entry in Annex VI).

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: 2026-11-04.

[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: 2026-11-04.

[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: 2026-11-04.

[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: 2026-11-04.

[5] ISO. ISO 7010:2019 — Graphical symbols. Safety signs. URL: https://www.iso.org/standard/72424.html Accessed: 2026-11-04.

[6] ISO. ISO 3864-1:2011 — Safety colours and safety signs. URL: https://www.iso.org/standard/51021.html Accessed: 2026-11-04.

[7] PubChem. National Center for Biotechnology Information (NIH/NLM), chemical compound database. URL: https://pubchem.ncbi.nlm.nih.gov/compound/7824

[8] NIST. Chemistry WebBook, SRD 69. National Institute of Standards and Technology. URL: https://webbook.nist.gov/cgi/cbook.cgi?ID=106-70-7

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

[10] 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

[11] 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

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

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

[14] 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

[15] 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

[16] 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

[17] 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: 2026-11-04.

External links

NIST: https://webbook.nist.gov/cgi/cbook.cgi?ID=106-70-7

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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