SAFETY DATA SHEET (SDS)

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

Date: 10.11.2026 | Version: 9 | EN

n-hexane

hexane

CAS 110-54-3

C_6H_{14} | EC 203-777-6

MOLAR MASS	LOGP
86.18	3.9

HAZARD CLASSIFICATION (GHS / CLP)



Danger

H225 | H361f | H304 | H372 | H315 | H336 | H411

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	n-hexane
1.1 IUPAC name	hexane
1.1 CAS number	110-54-3
1.1 EC number	203-777-6
1.1 PubChem CID	8058
1.1 InChIKey	VLKZOEOYAKHREP-UHFFFAOYSA-N
1.1 SMILES	CCCCCC
1.1 Molecular formula	C_6H_{14} [7]
1.1 Molar mass	86.18 g/mol [7]
1.1 Exact mass	86.1096 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:



Danger

Hazard statements (H) [3][4][12]

H225	Highly flammable liquid and vapour
H361f	Suspected of damaging fertility
H304	May be fatal if swallowed and enters airways
H336	May cause drowsiness or dizziness
H372	Causes damage to organs through prolonged or repeated exposure
H315	Causes skin irritation
H411	Toxic to aquatic life with long lasting effects

Precautionary statements (P) [3][4][12]

P201	Obtain special instructions before use
P202	Do not handle until all safety precautions have been read and understood
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
P260	Do not breathe dust/fume/gas/mist/vapours/spray
P264	Wash thoroughly after handling
P271	Use only outdoors or in a well-ventilated area
P273	Avoid release to the environment
P280	Wear protective gloves/protective clothing/eye protection/face protection
P301+P310	IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician
P302+P352	IF ON SKIN: Wash with plenty of water
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
P308+P313	IF exposed or concerned: Get medical advice/attention
P312	Call a POISON CENTER or doctor/physician if you feel unwell
P314	Get medical advice/attention if you feel unwell

WORKING DRAFT 工作草稿

P331	Do NOT induce vomiting
P332+P313	If skin irritation occurs: Get medical advice/attention
P370+P378	In case of fire: Use appropriate media to extinguish
P391	Collect spillage
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

NOTE: CMR substance — employment of pregnant and breastfeeding women in work harmful to health is prohibited (Polish Labour Code Art. 176 § 1; Council of Ministers Regulation of 3 April 2017, Journal of Laws 2017 item 796). [17][18]

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.

3. Composition/information on ingredients

Substance type	pure substance
CAS Number	110-54-3
EC number	203-777-6
Molecular formula	C_6H_{14}
Concentration	≥99% (typical reagent-grade purity — to be confirmed by the supplier's specification)
Clp index no	601-037-00-0

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][15]

Skin contact

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

Eye contact

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

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][15]

Symptoms and effects

cough, shortness of breath, headache, dizziness; skin redness and irritation. [3][12]

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).

WORKING DRAFT 工作草稿

5. Firefighting measures

Suitable extinguishing media	Alcohol-resistant foam, carbon dioxide (CO_2), dry chemical powder, water spray/mist. [1][2][15]
Unsuitable extinguishing media	Full/compact water jet (splashes and spreads the burning liquid, which floats on water). [1][2][15]
Specific hazards	Thermal decomposition products: CO, CO2. [16]
Advice for firefighters	Use self-contained breathing apparatus (SCBA). Full protective suit. [1][2][15]
Flash Point	-22°C [7]
Auto-ignition temperature	225°C [7]

6. Accidental release measures

Personal precautions	Use personal protective equipment (see Section 8). Avoid breathing vapours. [1][2][15]
Environmental precautions	Prevent entry into sewers, groundwater and surface water. [1][2][15]
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][15]
Related sections	8; 13

7. Handling and storage

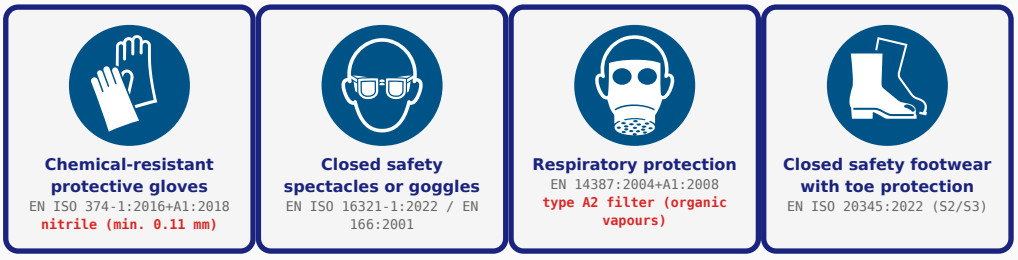
Precautions	Work in a fume hood or with adequate ventilation. No eating, drinking or smoking in the work area. [1][2][15]
Storage temperature	Store at room temperature (15-25°C) or as indicated on the label. [1][2][15]
Humidity	Store in a dry place (<60% RH). [1][2][15]
Light	Protect from direct sunlight. [1][2][15]
Incompatible materials	Strong oxidizers, Ignition sources, open flames. [16]

8. Exposure controls/personal protection

8.1 Control parameters

OEL — NDS (Poland)	NDS = 72 mg/m³ (TWA) — Rozp. MRiPS Dz.U.2024 poz.1017 [26]
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][19]



9. Physical and chemical properties

Property (item 9.1)	Value	Source
Physical state	Liquid	

WORKING DRAFT 工作草稿

Property (item 9.1)	Value	Source
Colour	Liquid [7]	
Odour	Gasoline-like odor [7]	
pH (1% aqueous solution)	Not applicable	
Melting point	-95.32°C [8] [7][24]	
Boiling point	68.7771°C [8] [7][24]	
Flash point	-22°C (experimental data) [7]	
Flammability	Flam. Liq. 2 (H225) [3][12]	
Lower and upper explosion limit	1–8.9 % obj. [24]	
Density (20°C)	0.6595 g/cm³ [7][24]	
Vapour pressure	15.999 kPa (120 mmHg, 20°C) [7][24]	
Relative vapour density	2.97 [23]	
Dynamic viscosity	0.377 mPa·s [7]	
Kinematic viscosity	No data available.	
Refractive index nD²⁰	1.3727 (experimental data) [7]	
Auto-ignition temperature	225°C [7]	
Decomposition temperature	Not applicable	
Surface Tension	17.89 mN/m [9]	
Water solubility	0.013 g/L, 20°C [7]	
Particle characteristics	Not applicable (REACH 9.1(r))	
Partition coefficient n-octanol/water (log value)	3.9 [25]	
Molar mass	86.18 g/mol [7]	
Molecular formula	C_6H_{14} [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)	25000 mg/kg (rat) [10]
LD50 (dermal)	No data available.
LC50 (inhalation)	LC50 169000 mg/m3 (rat) [11][12]
Skin irritation	Category 2 — skin irritation.

WORKING DRAFT · 工作草稿

Eye irritation	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][12]
Sensitisation	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][12]
Mutagenicity	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][12]
Carcinogenicity	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][12]
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	Category 2 (harmonised classification, Annex VI to CLP).
STOT — single exposure	Category 3 (H336): May cause drowsiness or dizziness. [3][12]
STOT — repeated exposure	Category 1 (H372): Causes damage to organs through prolonged or repeated exposure. [3][12]
Aspiration hazard	Category 1 (H304): May be fatal if swallowed and enters airways. [3][12]

12. Ecological information

Aquatic toxicity	Harmonised classification (CLP Annex VI): H411 — Toxic to aquatic life with long lasting effects (Aquatic Chronic 2). LC_{50} (fish): 2.5 mg/L (Pimephales promelas, 96 h) [22]
Persistence / biodegradability	No data available.
Bioaccumulative potential	log Kow = 3.9. Low bioaccumulation potential (log Kow < 4.5 — PBT/vPvB screening criterion per ECHA Guidance R.11). [20][21]
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. [14]
Packaging	Cleaned packaging may be recycled. Contaminated packaging must be treated as hazardous waste.

14. Transport information



Class 3 — Flammable liquids

UN number	UN 1208 [13]
Proper shipping name	Hexanes [13]
Transport hazard class	3 [13]
Packing Group	II [13]
Environmental hazard	CLP classification (H411) indicates aquatic environmental hazard — marine pollutant marking may be required; confirm per ADR 2.2.9 / IMDG criteria [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.

WORKING DRAFT 工作稿

Notes	Transport classification per ADR / UN Model Regulations (UN number, class and packing group above). Verify the ADR/IMDG/IATA edition in force on the date of shipment. [13]
Environmentally hazardous (mark: fish and tree)	Yes

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 10.11.2026 were omitted as future (not yet applicable).

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

Scientific citations (10)

et al.. *Assessment of CPME as Sustainable Low VOC Alternative to Hexane: Optimization of Extraction Efficiency and Bioactive Compound Yield from Fenugreek Seed Oil Using Computational and Experimental Methods.*. (2024). DOI: 10.3390/foods13233899

et al.. *Confined growth of UiO-66 into ultrahigh-loading membranes for efficient hexane isomer separation.*. (2025). DOI: 10.1039/d5sc04212g

Api AM, Belsito D, Botelho D et al.. *RIFM fragrance ingredient safety assessment, n-hexane, CAS Registry Number 110-54-3.*. Food and chemical toxicology : an international journal published for the British Industrial Biological Research Association (2022). DOI: 10.1016/j.fct.2022.112973

et al.. *Comparative metabolic profiling, enzyme inhibitory activities, and in-silico analysis of the hexane extract and the hydrodistilled oil of Boswellia serrata.*. (2026). DOI: 10.1371/journal.pone.0348178

et al.. *Extraction of Phospholipids From Crude Rapeseed Oil by n-Hexane/Alcohol System: Effects of Solvent Composition on Extraction Performance and Oil Quality.*. (2026). DOI: 10.1002/fsn3.71866

Full text of H statements

H225	Highly flammable liquid and vapour
H361f	Suspected of damaging fertility
H304	May be fatal if swallowed and enters airways
H336	May cause drowsiness or dizziness
H372	Causes damage to organs through prolonged or repeated exposure
H315	Causes skin irritation
H411	Toxic to aquatic life with long lasting effects

Full text of P statements

P201	Obtain special instructions before use
P202	Do not handle until all safety precautions have been read and understood
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
P260	Do not breathe dust/fume/gas/mist/vapours/spray
P264	Wash thoroughly after handling
P271	Use only outdoors or in a well-ventilated area
P273	Avoid release to the environment

WORKING DRAFT 工作草稿

P280	Wear protective gloves/protective clothing/eye protection/face protection
P301+P310	IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician
P302+P352	IF ON SKIN: Wash with plenty of water
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
P308+P313	IF exposed or concerned: Get medical advice/attention
P312	Call a POISON CENTER or doctor/physician if you feel unwell
P314	Get medical advice/attention if you feel unwell
P331	Do NOT induce vomiting
P332+P313	If skin irritation occurs: Get medical advice/attention
P370+P378	In case of fire: Use appropriate media to extinguish
P391	Collect spillage
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)
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

v9 (10.11.2026)	Based on ECHA harmonised classification (Annex VI to CLP, ATP 23).

WORKING DRAFT 工作草稿

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: 2026-11-10.

[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: 2026-11-10.

[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: 2026-11-10.

[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: 2026-11-10.

[5] ISO. ISO 7010:2019 — Graphical symbols. Safety signs. URL: https://www.iso.org/standard/72424.html Accessed: 2026-11-10.

[6] ISO. ISO 3864-1:2011 — Safety colours and safety signs. URL: https://www.iso.org/standard/51021.html Accessed: 2026-11-10.

[7] PubChem. National Center for Biotechnology Information (NIH/NLM), chemical compound database. URL: https://pubchem.ncbi.nlm.nih.gov/compound/8058

[8] NIST. Chemistry WebBook, SRD 69. National Institute of Standards and Technology. URL: https://webbook.nist.gov/cgi/cbook.cgi?ID=110-54-3

[9] Reid, R.C., Prausnitz, J.M., Poling, B.E. The Properties of Gases and Liquids. 4th ed. New York: McGraw-Hill, 1987.

[10] NIOSH. Registry of Toxic Effects of Chemical Substances (RTECS). Cincinnati: NIOSH. URL: https://www.cdc.gov/niosh/rtecs

[11] ECHA. REACH Registration Dossier (registered substance, acute toxicity study record). Helsinki: European Chemicals Agency. URL: https://echa.europa.eu/registration-dossier

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

[13] UNECE. European Agreement concerning the International Carriage of Dangerous Goods by Road (ADR), 2025 edition (ECE/TRANS/352). Geneva: United Nations. URL: https://unece.org/adr

[14] 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

[15] 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

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

[17] Act of 26 June 1974 — Labour Code (Poland), Art. 176 § 1. Journal of Laws 2023 item 1465. URL: https://isap.sejm.gov.pl

[18] Council of Ministers of the Republic of Poland. Regulation of 3 April 2017 on the list of arduous, hazardous or health-harmful work for pregnant and breastfeeding women. Journal of Laws 2017 item 796. URL: https://isap.sejm.gov.pl/isap.nsf/DocDetails.xsp?id=WDU20170000796

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

[20] 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

[21] 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

[22] U.S. EPA. ECOTOX Knowledgebase. Washington, DC: U.S. Environmental Protection Agency. URL: https://cfpub.epa.gov/ecotox/

[23] 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

[24] DECHEMA, PTB, and BAM. CHEMSAFE - Database of Evaluated Safety Characteristics for the Avoidance of Explosions. Frankfurt am Main: DECHEMA e.V.; Braunschweig/Berlin: Physikalisch-Technische Bundesanstalt and Bundesanstalt fur Materialforschung und -prufung. URL: https://www.chemsafe.ptb.de

[25] Sangster, J. "Octanol-Water Partition Coefficients of Simple Organic Compounds." Journal of Physical and Chemical Reference Data 18, no. 3 (1989): 1111-1229. URL: https://doi.org/10.1063/1.555833

[26] 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: 2026-11-10.

External links

NIST: https://webbook.nist.gov/cgi/cbook.cgi?ID=110-54-3

ChEMBL: https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL15939

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



Legal notice: This document was generated automatically from data provided by PubChem (NIH), ECHA, NIST WebBook, ChemSpider (RSC) and other public databases. It DOES NOT REPLACE an approved Safety Data Sheet (SDS) compliant with Regulation (EC) No 1907/2006 (REACH). Before using the substance, verify the data against the manufacturer's current SDS.

Generator: Document generated automatically from ECHA harmonised classification (Annex VI to CLP) and public physicochemical databases.
Author: www.MolGod.org — platform for automated safety data sheets (SDS).
Issue date: 10.11.2026 | Document version: 9

WORKING