# SAFETY DATA SHEET (SDS)

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

Date: 18.10.2026 | Version: 5 | EN

## (2H14)Methylcyclohexane

*1,1,2,2,3,3,4,4,5,5,6-undecadeuterio-6-(trideuteriomethyl)cyclohexane*

**CAS 10120-28-2**

$C_7H_{14}$

| MOLAR MASS | LOGP |
|---|---|
| 112.27 | 3.6 |

| TPSA |
|---|
| 0 Å² |

## HAZARD CLASSIFICATION (GHS / CLP)



**Danger**

H225 H304 H315 H336 H411

*Classification from aggregated ECHA C&L notifications (PubChem PUG-View); notifier consensus <75% — protective approach (all reported hazards). Requires 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** | (2H14)Methylcyclohexane |
| **1.1 IUPAC name** | 1,1,2,2,3,3,4,4,5,5,6-undecadeuterio-6-(trideuteriomethyl)cyclohexane |
| **1.1 CAS number** | 10120-28-2 |
| **1.1 EC number** | No data |
| **1.1 PubChem CID** | 524602 |
| **1.1 InChIKey** | UAEPNZWRGJTJPN-OBYKGMMLSA-N |
| **1.1 SMILES** | [2H]C1(C(C(C(C(C1([2H])[2H])([2H])[2H])([2H])C([2H])([2H])[2H])([2H])[2H])([2H])[2H])[2H] |
| **1.1 Molecular formula** | $C_7H_{14}$ [7] |
| **1.1 Molar mass** | 112.27 g/mol [7] |
| **1.1 Exact mass** | 112.1974 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]

| | |
|---|---|
| **H225** | Highly flammable liquid and vapour |
| **H304** | May be fatal if swallowed and enters airways |
| **H315** | Causes skin irritation |
| **H336** | May cause drowsiness or dizziness |
| **H411** | Toxic to aquatic life with long lasting effects |

### 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 |
| **P261** | Avoid breathing 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 |
| **P312** | Call a POISON CENTER or doctor/physician 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 |

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| | |
|---|---|
| **P405** | Store locked up |
| **P501** | Dispose of contents/container to an approved waste collection point |

**Classification from aggregated ECHA C&L notifications (PubChem PUG-View); notifier consensus <75% — protective approach (all reported hazards). Requires verification against the official source (ECHA C&L / manufacturer's data sheet).**

## 3. Composition/information on ingredients

| | |
|---|---|
| **Substance type** | pure substance |
| **CAS Number** | 10120-28-2 |
| **Molecular formula** | $C_7H_{14}$ |
| **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

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

## 6. Accidental release measures

| | |
|---|---|
| **Personal precautions** | Use personal protective equipment (see Section 8). Avoid breathing dust/vapours. [1][2][11] |
| **Environmental precautions** | Prevent entry into sewers, groundwater and surface water. [1][2][11] |
| **Methods for containment and cleaning up** | Absorb with inert material (sand, vermiculite, diatomaceous earth) and collect into sealed, labelled containers. Do not release into drains. [1][2][11] |
| **Related sections** | 8; 13 |

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## 7. Handling and storage

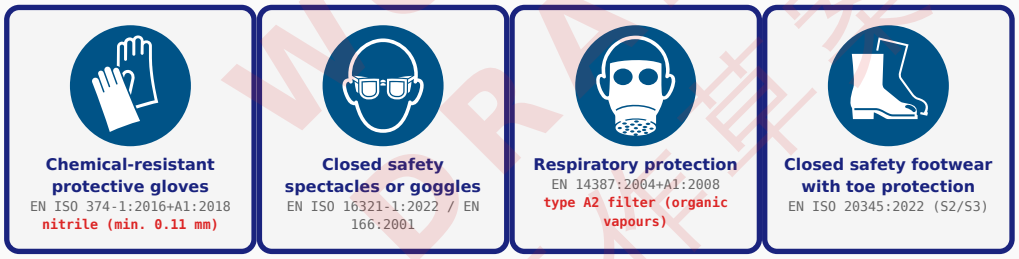
| | |
|---|---|
| **Precautions** | Work in a fume hood or with adequate ventilation. No eating, drinking or smoking in the work area. [1][2][11] |
| **Storage temperature** | Store at room temperature (15-25°C) or as indicated on the label. [1][2][11] |
| **Humidity** | Store in a dry place (<60% RH). [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** | No data available. | |
| **Colour** | No data available. | |
| **Odour** | No data available. | |
| **pH (1% aqueous solution)** | No data available. | |
| **Melting point** | No data available. | |
| **Boiling point** | No data available. | |
| **Flash point** | No data available. | |
| **Flammability** | Flam. Liq. 2 (H225) [3] | |
| **Lower and upper explosion limit** | No data available. | |
| **Density (20°C)** | No data available. | |
| **Vapour pressure** | No data available. | |
| **Relative vapour density** | No data available. | |
| **Kinematic viscosity** | No data available. | |

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| Property (item 9.1) | Value | Source |
|---|---|---|
| **Auto-ignition temperature** | No data available. | |
| **Decomposition temperature** | Not applicable | |
| **Water solubility** | No data available. | |
| **Particle characteristics** | No data available. | |
| **Partition coefficient n-octanol/water (log value)** | 3.6 [8] | |
| **Molar mass** | 112.27 g/mol [7] ✓86% | *PubChem* |
| **Molecular formula** | $C_7H_{14}$ [7] ✓86% | *PubChem* |
| **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** | Category 2 — skin irritation. |
| **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** | Category 3 (H336): May cause drowsiness or dizziness. [3] |
| **STOT — repeated exposure** | No data available. |
| **Aspiration hazard** | Category 1 (H304): May be fatal if swallowed and enters airways. [3] |

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## 12. Ecological information

| | |
|---|---|
| **Aquatic toxicity** | Classification per ECHA C&L notifications (self-classification, Art. 4(3)): H411 — Toxic to aquatic life with long lasting effects (Aquatic Chronic 2). Numerical $LC_{50}$/$EC_{50}$ data unverified in the available dataset — do not assume absence of toxicity. |
| **Persistence / biodegradability** | No data available. |
| **Bioaccumulative potential** | log Kow = 3.6 [8]. 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** | VERIFICATION REQUIRED — no verified UN assignment. |
| **Transport hazard class** | Suggested from GHS classification — VERIFICATION REQUIRED. |
| **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. |
| **Notes** | NOTE: the GHS classification indicates the substance may be subject to dangerous goods transport regulations (ADR/IMDG/IATA). Do NOT assume absence of restrictions — verify the UN number before shipping. |
| **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] |

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## 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 17.10.2026 were omitted as future (not yet applicable).

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

### Scientific citations (10)


Bryan W. Weber, WIlliam J. Pitz, Marco Mehl et al.. *Experiments and Modeling of the Autoignition of Methylcyclohexane at High Pressure*. arXiv (1706.02996v1) (2017). DOI: 10.1016/j.combustflame.2014.01.018

Víctor Alonso, Mario García, Juan Antonio González et al.. *Thermodynamics of mixtures containing alkoxyethanols. XXVIII: Liquid-liquid equilibria for 2-phenoxyethanol + selected alkanes*. arXiv (2402.05987v1) (2024). DOI: 10.1016/j.tca.2011.04.012

Shahram Ranjbar, Seyyed Hamid Momenian. *Densities and Viscosities of Binary and Ternary Mixtures of (Nitrobenzene + 1-Bromobutane), (1-Bromobutane + Methylcyclohexane), (Nitrobenzene + Methylcyclohexane), and (Methylcyclohexane + Nitrobenzene + 1-Bromobutane) from (293.15 to 308.15) K*. Journal of Chemical & Engineering Data (2011). DOI: 10.1021/je200350a

S. Zeppieri, K. Brezinsky, I. Glassman. *Pyrolysis studies of methylcyclohexane and oxidation studies of methylcyclohexane and methylcyclohexane/toluene blends*. Combustion and Flame (1997). DOI: 10.1016/s0010-2180(96)00125-3

Lei Wang, Peng Bai. *Isobaric vapor–liquid equilibrium data for methylcyclohexane+2-methoxyethanol and methylcyclohexane+2-ethoxyethanol at 50.00 and 101.33kPa*. Fluid Phase Equilibria (2014). DOI: 10.1016/j.fluid.2014.07.041


### Full text of H statements

| | |
|---|---|
| **H225** | Highly flammable liquid and vapour |
| **H304** | May be fatal if swallowed and enters airways |
| **H315** | Causes skin irritation |
| **H336** | May cause drowsiness or dizziness |
| **H411** | Toxic to aquatic life with long lasting effects |

### 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 |
| **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 |
| **P312** | Call a POISON CENTER or doctor/physician 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 |

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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 |

## Version history

| | |
|---|---|
| **v5 (17.10.2026)** | 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: 2026-10-17.

[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: 2026-10-17.

[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: 2026-10-17.

[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: 2026-10-17.

[5] ISO. ISO 7010:2019 — Graphical symbols. Safety signs. URL: https://www.iso.org/standard/72424.html Accessed: 2026-10-17.

[6] ISO. ISO 3864-1:2011 — Safety colours and safety signs. URL: https://www.iso.org/standard/51021.html Accessed: 2026-10-17.

[7] PubChem. National Center for Biotechnology Information (NIH/NLM), chemical compound database. URL: https://pubchem.ncbi.nlm.nih.gov/compound/524602

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

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

[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

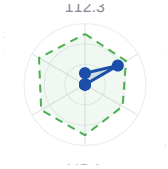
[16] MRiPS Regulation of 12.06.2018 — NDS/NDN. Journal of Laws 2024 item 1017. URL: https://isap.sejm.gov.pl/isap.nsf/DocDetails.xsp?id=WDU20240001017 Accessed: 2026-10-17.


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## External links

NIST: https://webbook.nist.gov/cgi/cbook.cgi?ID=10120-28-2

**ADMET / Drug-likeness**



**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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**Author:** www.MolGod.org — platform for automated safety data sheets (SDS).
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