SAFETY DATA SHEET (SDS)

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

Date: 05.11.2026 | Version: 9 | EN

3,5,5-trimethylcyclohex-2-enone

3,5,5-trimethylcyclohex-2-en-1-one

CAS 78-59-1

$C_9H_{14}O$ | EC 201-126-0

MOLAR MASS	LOGP
138.21	1.6

HAZARD CLASSIFICATION (GHS / CLP)



Warning

H351 | H312 | H302 | H335 | H319

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	3,5,5-trimethylcyclohex-2-enone
1.1 IUPAC name	3,5,5-trimethylcyclohex-2-en-1-one
1.1 CAS number	78-59-1
1.1 EC number	201-126-0
1.1 PubChem CID	6544
1.1 InChIKey	HJOVHMDZYOCNQW-UHFFFAOYSA-N
1.1 SMILES	CC1=CC(=O)CC(C1)(C)C
1.1 Molecular formula	$C_9H_{14}O$ [7]
1.1 Molar mass	138.21 g/mol [7]
1.1 Exact mass	138.1045 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]

H351	Suspected of causing cancer
H312	Harmful in contact with skin
H302	Harmful if swallowed
H335	May cause respiratory irritation
H319	Causes serious eye irritation

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

P201	Obtain special instructions before use
P202	Do not handle until all safety precautions have been read and understood
P261	Avoid breathing dust/fume/gas/mist/vapours/spray
P264	Wash thoroughly after handling
P270	Do not eat, drink or smoke when using this product
P271	Use only outdoors or in a well-ventilated area
P280	Wear protective gloves/protective clothing/eye protection/face protection
P301+P312	IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
P302+P352	IF ON SKIN: Wash with plenty of water
P304+P340	IF INHALED: Remove person to fresh air and keep comfortable for breathing
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes; Remove contact lenses, if present and easy to do. Continue rinsing
P308+P313	IF exposed or concerned: Get medical advice/attention
P312	Call a POISON CENTER or doctor/physician if you feel unwell
P330	Rinse mouth
P337+P313	If eye irritation persists: Get medical advice/attention
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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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). [15][16]

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	78-59-1
EC number	201-126-0
Molecular formula	$C_9H_{14}O$
Concentration	≥99% (typical reagent-grade purity — to be confirmed by the supplier's specification)
Clp index no	606-012-00-8
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][13]

Skin contact

Remove contaminated clothing. Rinse skin with soap and water (min. 15 minutes). Call a physician immediately. [1][2][13]

Eye contact

Rinse eyes with running water (min. 15 minutes). Remove contact lenses if possible. If irritation persists — consult an ophthalmologist. [1][2][13]

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][13]

Symptoms and effects

nausea, vomiting, diarrhoea; cough, shortness of breath, headache, dizziness; eye irritation and watering. [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).

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5. Firefighting measures

Suitable extinguishing media	Adapt extinguishing media to surroundings. CO2, dry powder, foam.
Unsuitable extinguishing media	No specific restrictions.
Specific hazards	Thermal decomposition products: CO, CO2. [14]
Advice for firefighters	Use self-contained breathing apparatus (SCBA). Full protective suit.
Flash Point	84°C [7]
Auto-ignition temperature	462.2°C [7]

6. Accidental release measures

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

7. Handling and storage

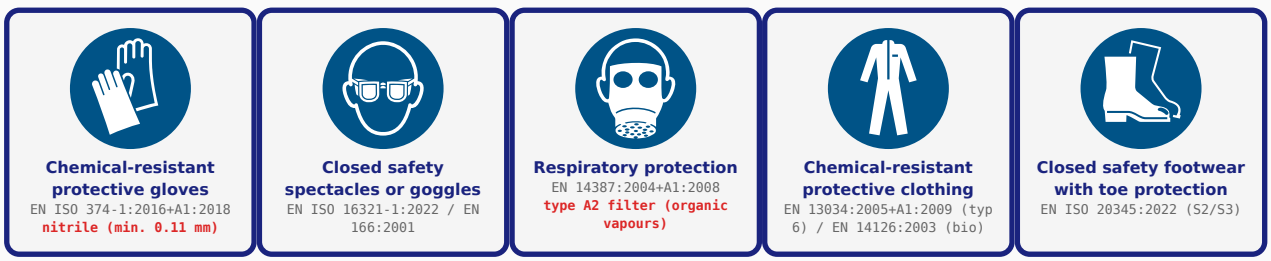
Precautions	Work in a fume hood or with adequate ventilation. No eating, drinking or smoking in the work area. [1][2][13]
Storage temperature	Store at room temperature (15-25°C) or as indicated on the label. [1][2][13]
Humidity	Store in a dry place (<60% RH). [1][2][13]
Light	Protect from direct sunlight. [1][2][13]
Incompatible materials	Strong oxidizers. [14]

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][17]



9. Physical and chemical properties

Property (item 9.1)	Value	Source
Physical state	Liquid	

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Property (item 9.1)	Value	Source
Colour	Water-white liquid [7]	
Odour	No data available.	
pH (1% aqueous solution)	No data available.	
Melting point	-8.1°C (experimental data) [7]	
Boiling point	214.1623°C [8] [7]	
Flash point	84°C (experimental data) [7]	
Flammability	No data available.	
Lower and upper explosion limit	No data available.	
Density (20°C)	0.9215 g/cm³ [7]	
Vapour pressure	0.027 kPa (0.2 mmHg, 20°C) (experimental data) [7]	
Relative vapour density	4.77 [21]	
Dynamic viscosity	2.62 mPa·s [7]	
Kinematic viscosity	No data available.	
Refractive index nD^{20}	1.4766 (experimental data) [7]	
Auto-ignition temperature	462.2°C (experimental data) [7]	
Decomposition temperature	Not applicable	
Water solubility	12 g/L, 25°C [7]	
Particle characteristics	Not applicable (REACH 9.1(r))	
Partition coefficient n-octanol/water (log value)	1.6 [9]	
Molar mass	138.21 g/mol [7]	
Molecular formula	$C_9H_{14}O$ [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.
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	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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Eye irritation	Category 2 — eye irritation.
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	Category 2 (harmonised classification, Annex VI to CLP).
IARC classification (carcinogenicity)	No individual IARC monograph — NOTE: substance classified as carcinogenic per ECHA CLP; absence of an IARC entry does NOT mean absence of carcinogenicity.
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]
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	LC_{50} (fish): 138 mg/L (Pimephales promelas, 96 h). EC_{50} (algae): 105 mg/L (Skeletonema costatum, 96 h) [20]
Persistence / biodegradability	No data available.
Bioaccumulative potential	log Kow = 1.6 [9]. Low bioaccumulation potential (log Kow < 4.5 — PBT/vPvB screening criterion per ECHA Guidance R.11). [18][19]
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. [12]
Packaging	Cleaned packaging may be recycled. Contaminated packaging must be treated as hazardous waste.

14. Transport information

UN number	UN 1993 [7]
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]

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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).

Scientific citations (7)

et al.. *RIFM fragrance ingredient safety assessment, 4-(2-butenylidene)-3,5,5-trimethylcyclohex-2-en-1-one, CAS registry number 13215-88-8.*. (2020). DOI: 10.1016/j.fct.2020.111377

Ecotoxicity Profile and Ambient Water Quality Advisories for 2-Cyclohexen-1-one, 3,5,5-trimethyl-. (1989).

Zhou H, Zhai J, Gong H et al.. *Novel pyrrolidine-alkylamino-substituted dicyanoisophorone derivatives as near-infrared fluorescence probe for imaging β-amyloid in vitro and in vivo.*. Analytica chimica acta (2024). DOI: 10.1016/j.aca.2024.342894

Vidal DM, Moreira MAB, Coracini MDA et al.. *Isophorone derivatives as a new structural motif of aggregation pheromones in Curculionidae.*. Scientific reports (2019). DOI: 10.1038/s41598-018-37156-8

Logeshwari G, Jeyashri KR, Rajkumar M et al.. *Benzylidene-isophorone hybrids with strong anticancer activity.*. Spectrochimica acta. Part A, Molecular and biomolecular spectroscopy (2024). DOI: 10.1016/j.saa.2024.124577

Full text of H statements

H351	Suspected of causing cancer
H312	Harmful in contact with skin
H302	Harmful if swallowed
H335	May cause respiratory irritation
H319	Causes serious eye irritation

Full text of P statements

P201	Obtain special instructions before use
P202	Do not handle until all safety precautions have been read and understood
P261	Avoid breathing dust/fume/gas/mist/vapours/spray
P264	Wash thoroughly after handling
P270	Do not eat, drink or smoke when using this product
P271	Use only outdoors or in a well-ventilated area
P280	Wear protective gloves/protective clothing/eye protection/face protection
P301+P312	IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
P302+P352	IF ON SKIN: Wash with plenty of water
P304+P340	IF INHALED: Remove person to fresh air and keep comfortable for breathing
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes; Remove contact lenses, if present and easy to do. Continue rinsing
P308+P313	IF exposed or concerned: Get medical advice/attention
P312	Call a POISON CENTER or doctor/physician if you feel unwell
P330	Rinse mouth
P337+P313	If eye irritation persists: Get medical advice/attention
P403+P233	Store in a well-ventilated place: Keep container tightly closed
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P501	Dispose of contents/container to an approved waste collection point

Abbreviations

ADR	European Agreement concerning the International Carriage of Dangerous Goods by Road

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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 (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/6544

[8] NIST. Chemistry WebBook, SRD 69. National Institute of Standards and Technology. URL: https://webbook.nist.gov/cgi/cbook.cgi?ID=78-59-1

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

[12] 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

[13] 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

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

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

[16] 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

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

[18] 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

[19] 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

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

[21] 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

[22] 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=78-59-1

ChEMBL: https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL1882894

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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