

SAFETY DATA SHEET (SDS)

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

Date: 03.09.2026 | Version: 1 | EN

4-hydroxy-4-methylpentan-2-one; diacetone alcohol

4-hydroxy-4-methylpentan-2-one

CAS 123-42-2

C₆H₁₂O₂

EC 204-626-7

MOLAR MASS
116.16LOGP
-0.2

HAZARD CLASSIFICATION (GHS / CLP)



Warning

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	4-hydroxy-4-methylpentan-2-one; diacetone alcohol
1.1 IUPAC name	4-hydroxy-4-methylpentan-2-one
1.1 CAS number	123-42-2
1.1 EC number	204-626-7
1.1 PubChem CID	31256
1.1 InChIKey	SWXVUIWOUIDPGS-UHFFFAOYSA-N
1.1 SMILES	CC(=O)CC(C)(C)O
1.1 Molecular formula	C ₆ H ₁₂ O ₂ ^[7]
1.1 Molar mass	116.16 g/mol ^[7]
1.1 Exact mass	116.0837 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)

2. Hazards identification

GHS:



PPE:



Warning

Hazard statements (H) ^{[3][4][10]}

H319 Causes serious eye irritation

Precautionary statements (P) ^{[3][4][10]}

P264 Wash thoroughly after handling

P280 Wear protective gloves/protective clothing/eye protection/face protection

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes; Remove contact lenses, if present and easy to do. Continue rinsing

P337+P313 If eye irritation persists: Get medical advice/attention

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.

3. Composition/information on ingredients

Substance type	pure substance
CAS Number	123-42-2
EC number	204-626-7
Molecular formula	C ₆ H ₁₂ O ₂
Concentration	≥99% (typical reagent-grade purity — to be confirmed by the supplier's specification)
Clp index no	603-016-00-1
Specyficzne stężenia graniczne / M-współczynnik (CLP Zał. VI Tab.3)	SCL: H319: 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). ^{[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. Poison Centre Łódź: +48 42 631 47 24 (24/7). Emergency number: 112. ^{[1][2][13]}

Symptoms and effects

eye irritation and watering. ^{[3][10]}

Notes for physician

Requires verification

Emergency numbers: CIT Łódź: +48 42 631 47 24 (24/7) | Emergency: 112

5. Firefighting measures

Suitable extinguishing media	Adapt extinguishing media to surroundings. CO ₂ , dry powder, foam.
Unsuitable extinguishing media	No specific restrictions.
Specific hazards	Thermal decomposition products: CO, CO ₂ . ^[14]
Advice for firefighters	Use self-contained breathing apparatus (SCBA). Full protective suit.
Flash Point	8°C ^[7]
Auto-ignition temperature	603.3°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][15]}

 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	 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	No data available.	
pH (1% aqueous solution)	No data available.	
Melting point	-43.1923°C ^{[8] [7]}	
Boiling point	166.6885°C ^{[8] [7]}	
Flash point	8°C (experimental data) ^[7]	
Flammability	No data available.	
Lower and upper explosion limit	No data available.	
Density (20°C)	0.9346 g/cm ³ ^[7]	
Vapour pressure	0.129 kPa (0.97 mmHg, 20°C) (experimental data) ^[7]	
Relative vapour density	4.01 ^[19]	
Kinematic viscosity	No data available.	
Refractive index n_D²⁰	1.4232 (experimental data) ^[7]	
Auto-ignition temperature	603.3°C (experimental data) ^[7]	
Decomposition temperature	Not applicable	

Property (item 9.1)	Value	Source
Rozpuszcz. w wodzie	1000 g/L ^[7]	
Particle characteristics	Not applicable (REACH 9.1(r))	
Partition coefficient n-octanol/water (log value)	-0.2 ^[9]	
Molar mass	116.16 g/mol ^[7]	
Molecular formula	C ₆ H ₁₂ 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.
Decomposition products	Thermal decomposition products:CO, CO ₂ .

11. Toxicological information

LD50 (oral)	LD50 4.0 g/kg (rat, oral) ^[7]
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]}
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	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	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) ^{[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): 420 mg/L (Lepomis macrochirus, 96 h). EC ₅₀ (Daphnia): 8750 mg/L (Daphnia magna, 24 h) ^[18]
Persistence / biodegradability	No data available.
Bioaccumulative potential	log Kow = -0.2 ^[9] . Low bioaccumulation potential (log Kow < 4.5 — PBT/vPvB screening criterion per ECHA Guidance R.11). ^{[16][17]}
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 (np. chemical reagents) zawierające substancje niebezpieczne. EWC code verification required. ^[12]
Packaging	Cleaned packaging may be recycled. Contaminated packaging must be treated as hazardous waste.

14. Transport information

UN number	UN 1148 ^[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]
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 03.09.2026 were omitted as future (not yet applicable).

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

Scientific citations (10)

- Tan Y, Li D, Hua J et al.. Localization of a defensive volatile 4-hydroxy-4-methylpentan-2-one in the capitate glandular trichomes of *Oenothera glazioviana*. Plant diversity (2017). DOI: 10.1016/j.pld.2017.05.004
- I. Cibulka, L. Hnědkovský, J.-C. Fontaine et al.. Volumetric Properties of the Mixture 4-Methylpentan-2-one C₆H₁₂O + C₆H₁₂O₂ 4-Hydroxy-4-methylpentan-2-one (LB2753, VMDS1111). Landolt-Börnstein - Group IV Physical Chemistry (2009). DOI: 10.1007/978-3-540-73584-7_1520
- I. Cibulka, L. Hnědkovský, J.-C. Fontaine et al.. Volumetric Properties of the Mixture 4-Methylpentan-2-one C₆H₁₂O + C₆H₁₂O₂ 4-Hydroxy-4-methylpentan-2-one (LB2764, VMDS1212). Landolt-Börnstein - Group IV Physical Chemistry (2009). DOI: 10.1007/978-3-540-73584-7_1521
- Fadila Salhi, Nawel Cheikh, Didier Villemin et al.. Synthesis of 2-aminopyridine Lactones and Studies of Their Antioxidant, Antibacterial and Antifungal Properties. Chemistry Proceedings (2021). DOI: 10.3390/ecsoc-25-11709
- Christian Wohlfarth. Refractive index of 4-hydroxy-4-methylpentan-2-one. Optical Constants (2017). DOI: 10.1007/978-3-662-49236-9_239

Full text of H statements

H319 Causes serious eye irritation

Full text of P statements

P264 Wash thoroughly after handling

P280 Wear protective gloves/protective clothing/eye protection/face protection

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes; Remove contact lenses, if present and easy to do. Continue rinsing

P337+P313 If eye irritation persists: Get medical advice/attention

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

v1 (03.09.2026) 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: 2026-09-03.
- [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: 2026-09-03.
- [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: 2026-09-03.
- [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: 2026-09-03.
- [5] ISO. ISO 7010:2019 — Graphical symbols. Safety signs. URL: <https://www.iso.org/standard/72424.html> Accessed: 2026-09-03.
- [6] ISO. ISO 3864-1:2011 — Safety colours and safety signs. URL: <https://www.iso.org/standard/51021.html> Accessed: 2026-09-03.

- [7] PubChem. National Center for Biotechnology Information (NIH/NLM), chemical compound database. URL: <https://pubchem.ncbi.nlm.nih.gov/compound/31256>
- [8] NIST. Chemistry WebBook, SRD 69. National Institute of Standards and Technology. URL: <https://webbook.nist.gov/cgi/cbook.cgi?ID=123-42-2>
- [9] Rumble, J.R., ed. CRC Handbook of Chemistry and Physics. 105th ed. Boca Raton: CRC Press, 2024. URL: <https://hbcpc.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] CEN. Personal protective equipment standards (EN ISO 374-1, EN 166, EN 149, EN 14387, EN ISO 20345). Brussels: European Committee for Standardization.
- [16] 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>
- [17] 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>
- [18] U.S. EPA. ECOTOX Knowledgebase. Washington, DC: U.S. Environmental Protection Agency. URL: <https://cfpub.epa.gov/ecotox/>
- [19] 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>
- [20] 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: 2026-09-03.

External links

NIST: <https://webbook.nist.gov/cgi/cbook.cgi?ID=123-42-2>
ChEMBL: https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL3182048

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), Wikidata 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: 03.09.2026 | Document version: 1