SAFETY DATA SHEET (SDS)

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

Date: 21.10.2026 | Version: 5 | EN

benzaldehyde

benzaldehyde

CAS 100-52-7

C_7H_6O | EC 202-860-4

MOLAR MASS	LOGP
106.12	1.5

HAZARD CLASSIFICATION (GHS / CLP)



Warning

H302

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	benzaldehyde
1.1 IUPAC name	benzaldehyde
1.1 CAS number	100-52-7
1.1 EC number	202-860-4
1.1 PubChem CID	240
1.1 InChIKey	HUMNYLRZRPPJDN-UHFFFAOYSA-N
1.1 SMILES	C1=CC=C(C=C1)C=O
1.1 Molecular formula	C_7H_6O [7]
1.1 Molar mass	106.12 g/mol [7]
1.1 Exact mass	106.0419 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]

H302	Harmful if swallowed

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

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
P301+P312	IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
P330	Rinse mouth
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.

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3. Composition/information on ingredients

Substance type	pure substance
CAS Number	100-52-7
EC number	202-860-4
Molecular formula	C_7H_6O
Concentration	≥99% (typical reagent-grade purity — to be confirmed by the supplier's specification)
Clp index no	605-012-00-5

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. 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. [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).

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	62.8°C [7]
Auto-ignition temperature	192.2°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

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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][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]



9. Physical and chemical properties

Property (item 9.1)	Value	Source
Physical state	Liquid	
Colour	Strongly refractive liquid, becoming yellowish on keeping [7]	
Odour	Characteristic odor of volatile oil of almond [7]	
pH (1% aqueous solution)	No data available.	
Melting point	-36.3085°C [8] [7]	
Boiling point	178.8346°C [8] [7][20]	
Flash point	62.8°C (experimental data) [7]	
Flammability	No data available.	
Lower and upper explosion limit	No data available.	
Density (20°C)	1.046 g/cm³ [7][20]	
Vapour pressure	0.169 kPa (1.27 mmHg, 25°C) (experimental data) [7]	

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Property (item 9.1)	Value	Source
Relative vapour density	3.66 [19]	
Dynamic viscosity	1.321 mPa·s [7]	
Kinematic viscosity	No data available.	
Refractive index nD²⁰	1.5456 (experimental data) [7]	
Auto-ignition temperature	192.2°C [7]	
Decomposition temperature	Not applicable	
Water solubility	6.95 g/L, 25°C [7][21]	
Particle characteristics	Not applicable (REACH 9.1(r))	
Partition coefficient n-octanol/water (log value)	1.5 [9][22]	
Molar mass	106.12 g/mol [7]	
Molecular formula	C_7H_6O [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)	LD50 1430 mg/kg (rat, oral) [7]
LD50 (dermal)	LD50 >1250 mg/kg (rabbit) [7]
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	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10]
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]

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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): 1.07 mg/L (Lepomis macrochirus, 96 h). EC_{50} (algae): 0.028 mg/L (Chlorella vulgaris, 72 h) [18]
Persistence / biodegradability	No data available.
Bioaccumulative potential	log Kow = 1.5 [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 (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 1990 [7]
Environmental hazard	The aquatic hazard classes are not covered by the harmonised entry in Annex VI. Data in Section 12 indicate a value below the classification threshold — supplier self-classification (Article 4(3) CLP) and verification per ADR 2.2.9 / IMDG are required. Do not assume that marking as a marine pollutant is not 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]
Environmentally hazardous (mark: fish and tree)	Requires verification

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 21.10.2026 were omitted as future (not yet applicable).

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

Scientific citations (9)

Api AM, Belsito D, Biserta S et al.. *RIFM fragrance ingredient safety assessment, benzaldehyde, CAS Registry Number 100-52-7.*. Food and chemical toxicology : an international journal published for the British Industrial Biological Research Association (2019). DOI: 10.1016/j.fct.2019.110878

Talita Odriane Custodio Leite. *Benzaldehyde (CAS 100-52-7)*. Revista Virtual de Química (2020). DOI: 10.21577/1984-6835.20200015

Saito J, Onishi N, Yamasaki J et al.. *Benzaldehyde suppresses epithelial-mesenchymal plasticity and overcomes treatment resistance in cancer by targeting the interaction of 14-3-3ζ with H3S28ph.*. British journal of cancer (2025). DOI: 10.1038/s41416-025-03006-4

A mechanistic Study of the electrochemical reaction between nitrostyrene and benzaldehyde; DFT calculations on all possible routes and intermediates.. (2024). DOI: 10.21203/rs.3.rs-4684231/v1

Norris EJ, Kline J, Bloomquist JR. *Repellency and Toxicity of Vapor-Active Benzaldehydes against Aedes aegypti.*. ACS infectious diseases (2024). DOI: 10.1021/acsinfecdis.3c00294

Full text of H statements

H302	Harmful if swallowed

Full text of P statements

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
P301+P312	IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
P330	Rinse mouth
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

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Version history

v5 (21.10.2026)	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: 2026-10-21.

[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: 2026-10-21.

[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: 2026-10-21.

[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: 2026-10-21.

[5] ISO. ISO 7010:2019 — Graphical symbols. Safety signs. URL: https://www.iso.org/standard/72424.html Accessed: 2026-10-21.

[6] ISO. ISO 3864-1:2011 — Safety colours and safety signs. URL: https://www.iso.org/standard/51021.html Accessed: 2026-10-21.

[7] PubChem. National Center for Biotechnology Information (NIH/NLM), chemical compound database. URL: https://pubchem.ncbi.nlm.nih.gov/compound/240

[8] NIST. Chemistry WebBook, SRD 69. National Institute of Standards and Technology. URL: https://webbook.nist.gov/cgi/cbook.cgi?ID=100-52-7

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

[10] 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] 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

[21] NLM. Hazardous Substances Data Bank (HSDB). National Library of Medicine. URL: https://www.nlm.nih.gov

[22] 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

[23] 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: 2026-10-21.

External links

NIST: https://webbook.nist.gov/cgi/cbook.cgi?ID=100-52-7

ChEMBL: https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL15972

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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