SAFETY DATA SHEET (SDS)

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

Date: 23.09.2026 | Version: 1 | EN

octan butylu

butyl acetate

CAS 123-86-4

$C_6H_{12}O_2$ | EC 204-658-1

易 普 化 工
EAPEARL CHEM

MOLAR MASS	LOGP
116.16	1.8

HAZARD CLASSIFICATION (GHS / CLP)



Warning

H226 | H336 | EUH066

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	octan butylu
1.1 IUPAC name	butyl acetate
1.1 CAS number	123-86-4
1.1 EC number	204-658-1
1.1 PubChem CID	31272
1.1 InChIKey	DKPFZGUDAPQIHT-UHFFFAOYSA-N
1.1 SMILES	CCCCOC(=O)C
1.1 Molecular formula	$C_6H_{12}O_2$ [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	+48 42 631 47 24

Toxicological Information Centre (CIT), Łódź — available 24/7

2. Hazards identification

GHS:



PPE:



Prohibitions:



Warning

Hazard statements (H) [3][4][9]

H226	Flammable liquid and vapour
H336	May cause drowsiness or dizziness
EUH066	Repeated exposure may cause skin dryness or cracking.

Precautionary statements (P) [3][4][9]

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
P271	Use only outdoors or in a well-ventilated area
P280	Wear protective gloves/protective clothing/eye protection/face protection
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
P370+P378	In case of fire: Use appropriate media to extinguish
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

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	123-86-4
EC number	204-658-1
Molecular formula	$C_6H_{12}O_2$
Concentration	≥99% (typical reagent-grade purity — to be confirmed by the supplier's specification)
Clp index no	607-025-00-1

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][12]

Skin contact

Remove contaminated clothing. Rinse skin with soap and water (min. 15 minutes). [1][2][12]

Eye contact

Rinse eyes with running water (min. 15 minutes). Remove contact lenses if possible. If irritation persists — consult an ophthalmologist. [1][2][12]

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][12]

Symptoms and effects

cough, shortness of breath, headache, dizziness. [3][9]

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][12]
Unsuitable extinguishing media	Full/compact water jet (splashes and spreads the burning liquid, which floats on water). [1][2][12]
Specific hazards	Thermal decomposition products:CO, CO2. [13]
Advice for firefighters	Use self-contained breathing apparatus (SCBA). Full protective suit. [1][2][12]
Flash Point	22°C [7]
Auto-ignition temperature	404.4°C [7]

6. Accidental release measures

Personal precautions	Use personal protective equipment (see Section 8). Avoid breathing vapours. [1][2][12]
Environmental precautions	Prevent entry into sewers, groundwater and surface water. [1][2][12]
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][12]
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][12]

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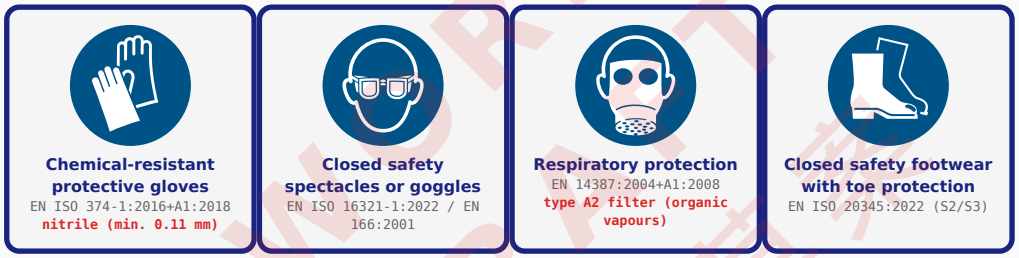
Storage temperature	Store at room temperature (15-25°C) or as indicated on the label. [1][2][12]
Humidity	Store in a dry place (<60% RH). [1][2][12]
Light	Protect from direct sunlight. [1][2][12]
Incompatible materials	Strong oxidizers, Ignition sources, open flames. [13]

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][14]



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)	Not applicable	
Melting point	-77.22°C [8] [7]	
Boiling point	125.9327°C [8] [7]	
Flash point	22°C (experimental data) [7]	
Flammability	Flam. Liq. 3 (H226) [3][9]	
Lower and upper explosion limit	No data available.	
Density (20°C)	0.8774 g/cm³ [7]	
Vapour pressure	1.333 kPa (10 mmHg, 20°C) (experimental data) [7]	
Relative vapour density	4.01 [18]	
Dynamic viscosity	0.685 mPa·s [7]	
Kinematic viscosity	No data available.	
Refractive index nD^{20}	1.3941 (experimental data) [7]	
Auto-ignition temperature	404.4°C (experimental data) [7]	

Property (item 9.1)	Value	Source
Decomposition temperature	Not applicable	
Rozpuszcz. w wodzie	14 g/L, 20°C [7]	
Particle characteristics	Not applicable (REACH 9.1(r))	
Partition coefficient n-octanol/water (log value)	1.8 [7]	
Molar mass	116.16 g/mol [7]	
Molecular formula	$C_6H_{12}O_2$ [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, Ignition sources, open flames.
Decomposition products	Thermal decomposition products:CO, CO2.

11. Toxicological information

LD50 (oral)	No data available.
LD50 (dermal)	LD50 >14112 mg/kg (rabbit) [7]
LC50 (inhalation)	LC50 390 ppm (4 h) (rat) [7]
Skin irritation	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][9]
Eye irritation	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][9]
Sensitisation	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][9]
Mutagenicity	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][9]
Carcinogenicity	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][9]
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][9]
STOT — single exposure	Category 3 (H336): May cause drowsiness or dizziness. [3][9]
STOT — repeated exposure	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][9]
Aspiration hazard	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][9]

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12. Ecological information

Aquatic toxicity	LC_{50} (fish): 18 mg/L (Pimephales promelas, 96 h). EC_{50} (Daphnia): 205 mg/L (Daphnia magna, 24 h) [17]
Persistence / biodegradability	No data available.
Bioaccumulative potential	log Kow = 1.8 [7]. Low bioaccumulation potential (log Kow < 4.5 — PBT/vPvB screening criterion per ECHA Guidance R.11). [15][16]
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) zawierajace substancje niebezpieczne. EWC code verification required. [11]
Packaging	Cleaned packaging may be recycled. Contaminated packaging must be treated as hazardous waste.

14. Transport information



Class 3 — Flammable liquids

UN number	UN 1123 [7]
Transport hazard class	Suggested from GHS classification — VERIFICATION REQUIRED.
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 after23.09.2026 were omitted as future (not yet applicable).

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

Scientific citations (10)

et al.. Comprehensive evaluation for the one-pot biosynthesis of butyl acetate by using microbial mono- and co-cultures.. (2021). DOI: 10.1186/s13068-021-02053-2

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Api AM, Belsito D, Botelho D et al.. RIFM fragrance ingredient safety assessment, butyl acetate, CAS Registry Number 123-86-4.. Food and chemical toxicology : an international journal published for the British Industrial Biological Research Association (2022). DOI: 10.1016/j.fct.2022.113439

et al.. Excess Enthalpies for Binary Mixtures of the Reactive System Acetic Acid + n-Butanol + n-Butyl Acetate + Water: Brief Data Review and Results at 313.15 K and Atmospheric Pressure.. (2023). DOI: 10.3390/ijms24065137

et al.. Synthesis of n-butyl acetate via reactive distillation column using Candida Antarctica lipase as catalyst.. (2020). DOI: 10.1007/s00449-019-02250-2

et al.. Combined effects of ultrasound and immobilization protocol on butyl acetate synthesis catalyzed by CALB.. (2014). DOI: 10.3390/molecules19079562

Full text of H statements

H226	Flammable liquid and vapour
H336	May cause drowsiness or dizziness
EUH066	Repeated exposure may cause skin dryness or cracking.

Full text of P statements

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P233	Keep container tightly closed
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P271	Use only outdoors or in a well-ventilated area
P280	Wear protective gloves/protective clothing/eye protection/face protection
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
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P370+P378	In case of fire: Use appropriate media to extinguish
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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

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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 (23.09.2026)	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: 2026-09-23.

[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: 2026-09-23.

[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: 2026-09-23.

[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: 2026-09-23.

[5] ISO. ISO 7010:2019 — Graphical symbols. Safety signs. URL: https://www.iso.org/standard/72424.html Accessed: 2026-09-23.

[6] ISO. ISO 3864-1:2011 — Safety colours and safety signs. URL: https://www.iso.org/standard/51021.html Accessed: 2026-09-23.

[7] PubChem. National Center for Biotechnology Information (NIH/NLM), chemical compound database. URL: https://pubchem.ncbi.nlm.nih.gov/compound/31272

[8] NIST. Chemistry WebBook, SRD 69. National Institute of Standards and Technology. URL: https://webbook.nist.gov/cgi/cbook.cgi?ID=123-86-4

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

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

[11] 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

[12] 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

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

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

[15] 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

[16] 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

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

[18] 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

[19] 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: 2026-09-23.

External links

NIST: https://webbook.nist.gov/cgi/cbook.cgi?ID=123-86-4

Wikidata: https://www.wikidata.org/wiki/Q411073

ChEMBL: https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL284391

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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