

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

butane-2,3-dione

butane-2,3-dione

CAS 431-03-8

 $C_4H_6O_2$ MOLAR MASS
86.09LOGP
-1.3

HAZARD CLASSIFICATION (GHS / CLP)



Danger

H225 H302 H315 H317 H318 H331 H373 H332 H335

Non-harmonised classification (no entry in Annex VI to CLP) — assigned from aggregated ECHA C&L notifications; the H-statements require 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

1.1 IUPAC name

butane-2,3-dione

1.1 CAS number

431-03-8

1.1 EC number

No data

1.1 PubChem CID

650

1.1 InChIKey

QSJXEFYPDANLFS-UHFFFAOYSA-N

1.1 SMILES

CC(=O)C(=O)C

1.1 Molecular formula

 $C_4H_6O_2$ ^[7]

1.1 Molar mass

86.09 g/mol ^[7]

1.1 Exact mass

86.0368 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



Danger

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

H225	Highly flammable liquid and vapour
H302	Harmful if swallowed
H315	Causes skin irritation
H317	May cause an allergic skin reaction
H318	Causes serious eye damage
H331	Toxic if inhaled
H373	May cause damage to organs through prolonged or repeated exposure
H332	Harmful if inhaled
H335	May cause respiratory irritation

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
P260	Do not breathe 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
P272	Contaminated work clothing should not be allowed out of the workplace
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
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
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes; Remove contact lenses, if present and easy to do. Continue rinsing
P310	Immediately call a POISON CENTER or doctor/physician
P311	Call a POISON CENTER or doctor/physician
P312	Call a POISON CENTER or doctor/physician if you feel unwell

P314	Get medical advice/attention if you feel unwell
P321	Specific treatment
P330	Rinse mouth
P332+P313	If skin irritation occurs: Get medical advice/attention
P333+P313	If skin irritation or rash occurs: Get medical advice/attention
P362+P364	Take off contaminated clothing
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

Non-harmonised classification (no entry in Annex VI to CLP) — assigned from aggregated ECHA C&L notifications; the H-statements require verification against the official source (ECHA C&L / manufacturer's data sheet).

3. Composition/information on ingredients

Substance type	pure substance
CAS Number	431-03-8
Molecular formula	C ₄ H ₆ O ₂
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. Call a physician. Semi-sitting position. Give oxygen if available. 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. Call an ophthalmologist immediately. ^{[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. Poison Centre Łódź: +48 42 631 47 24 (24/7). Emergency number: 112. ^{[1][2][11]}

Symptoms and effects

nausea, vomiting, diarrhoea; cough, shortness of breath, headache, dizziness; skin redness and irritation; eye irritation and watering. ^[3]

Notes for physician

Requires verification

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

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, CO ₂ . ^[12]
Advice for firefighters	Use self-contained breathing apparatus (SCBA). Full protective suit. ^{[1][2][11]}
Flash Point	6°C ^[7]
Auto-ignition temperature	365°C ^[7]

6. Accidental release measures

Personal precautions	Use personal protective equipment (see Section 8). Avoid breathing vapours. ^{[1][2][11]}
Environmental precautions	Prevent entry into sewers, groundwater and surface water. ^{[1][2][11]}
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][11]}
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][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]}



Chemical-resistant protective gloves
EN ISO 374-1:2016+A1:2018
butyl (type B/C) – NOT latex



Closed safety spectacles or goggles
EN ISO 16321-1:2022 / EN 166:2001



Respiratory protection
EN 14387:2004+A1:2008
type A2-P3 filter (organic vapours + particles)



Face shield (splash risk)
EN ISO 16321-1:2022



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	

Property (item 9.1)	Value	Source
Colour	No data available.	
Odour	No data available.	
pH (1% aqueous solution)	No data available.	
Melting point	-1.2°C (experimental data) ^[7]	
Boiling point	87.9038°C ^[8] ^[7]	
Flash point	6°C (experimental data) ^[7]	
Flammability	Flam. Liq. 2 (H225) ^[3]	
Lower and upper explosion limit	No data available.	
Density (20°C)	0.99 g/cm ³ ^[7]	
Vapour pressure	7.573 kPa (56.8 mmHg, 25°C) (experimental data) ^[7]	
Relative vapour density	2.97 ^[16]	
Kinematic viscosity	No data available.	
Refractive index n _D ²⁰	1.3951 (experimental data) ^[7]	
Auto-ignition temperature	365°C (experimental data) ^[7]	
Decomposition temperature	Not applicable	
Rozpuszcz. w wodzie	200 g/L, 20°C ^[7]	
Particle characteristics	Not applicable (REACH 9.1(r))	
Partition coefficient n-octanol/water (log value)	-1.3 ^[9]	
Molar mass	86.09 g/mol ^[7]	
Molecular formula	C ₄ H ₆ 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)	LD50 1580 mg/kg (rat, oral) ^[7]
LD50 (dermal)	No data available.
LC50 (inhalation)	No data available.
Skin irritation	Category 2 — skin irritation.
Eye irritation	Category 1 — serious eye damage.

Sensitisation	Skin, Category 1 (H317): May cause an allergic skin reaction. ^[3]
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 (H335): May cause respiratory irritation. ^[3]
STOT — repeated exposure	Category 2 (H373): May cause damage to organs through prolonged or repeated exposure. ^[3]
Aspiration hazard	No data available.

12. Ecological information

Aquatic toxicity	No data available.
Persistence / biodegradability	No data available.
Bioaccumulative potential	log Kow = -1.3 ^[9] . 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 (np. chemical reagents) zawierające substancje niebezpieczne. EWC code verification required. ^[10]
Packaging	Cleaned packaging may be recycled. Contaminated packaging must be treated as hazardous waste.

14. Transport information



Class 3 — Flammable liquids



Class 6.1 — Toxic substances

UN number	UN 2346 ^[7]
Transport hazard class	Suggested from GHS classification — VERIFICATION REQUIRED.
Environmental hazard	Environmental hazard for transport: not verified. Non-harmonised classification (outside CLP Annex VI) — verify aquatic toxicity (Section 12) and do NOT assume marine pollutant marking is not required; confirm per ADR 2.2.9 / IMDG before shipping.
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]

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 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)

Effah F, Taiwo B, Baines D et al.. Pulmonary effects of e-liquid flavors: a systematic review.. *Journal of toxicology and environmental health. Part B, Critical reviews* (2022). DOI: 10.1080/10937404.2022.2124563

Brass DM, Palmer SM. Models of toxicity of diacetyl and alternative diones.. *Toxicology* (2017). DOI: 10.1016/j.tox.2017.02.011

Hubbs AF, Kreiss K, Cummings KJ et al.. Flavorings-Related Lung Disease: A Brief Review and New Mechanistic Data.. *Toxicologic pathology* (2019). DOI: 10.1177/0192623319879906

Øyvind Eggen. Bistand som politisk markering. *Internasjonal Politikk* (2013). DOI: 10.18261/issn1891-1757-2013-03-09

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Full text of H statements

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Full text of P statements

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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

v1 (03.09.2026)	Based on supplier self-classification (ECHA C&L notifications; no harmonised entry in Annex VI).
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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.
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- [8] NIST. Chemistry WebBook, SRD 69. National Institute of Standards and Technology. URL: <https://webbook.nist.gov/cgi/cbook.cgi?ID=431-03-8>
- [9] Rumble, J.R., ed. CRC Handbook of Chemistry and Physics. 105th ed. Boca Raton: CRC Press, 2024. URL: <https://hbcpc.chemnetbase.com>
- [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>
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- [12] Urban, 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>
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- [16] 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>
- [17] 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=431-03-8>

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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