WORKING DRAFT · 工作草案

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

bezwodnik ftalowy

2-benzofuran-1,3-dione

CAS 85-44-9

$C_8H_4O_3$ | EC 201-607-5

易 普 化 工
EAPEARL CHEM

MOLAR MASS	LOGP
148.11	1.3

HAZARD CLASSIFICATION (GHS / CLP)



Danger

H302 | H335 | H315 | H318 | H334 | H317

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	bezwodnik ftalowy
1.1 IUPAC name	2-benzofuran-1,3-dione
1.1 CAS number	85-44-9
1.1 EC number	201-607-5
1.1 PubChem CID	6811
1.1 InChIKey	LGRFSURHDFAFJT-UHFFFAOYSA-N
1.1 SMILES	C1=CC=C2C(=C1)C(=O)OC2=O
1.1 Molecular formula	$C_8H_4O_3$ [7]
1.1 Molar mass	148.11 g/mol [7]
1.1 Exact mass	148.0160 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:



Danger

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

H302	Harmful if swallowed
H335	May cause respiratory irritation
H315	Causes skin irritation
H318	Causes serious eye damage
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled
H317	May cause an allergic skin reaction

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

P233	Keep container tightly closed
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
P272	Contaminated work clothing should not be allowed out of the workplace
P280	Wear protective gloves/protective clothing/eye protection/face protection
P284	Wear respiratory 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
P310	Immediately call a POISON CENTER or doctor/physician
P312	Call a POISON CENTER or doctor/physician 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

WORKING DRAFT · 工作稿

P342+P311	If experiencing respiratory symptoms: Call a POISON CENTER or doctor/ physician
P362+P364	Take off contaminated clothing
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.

3. Composition/information on ingredients

Substance type	pure substance
CAS Number	85-44-9
EC number	201-607-5
Molecular formula	$C_8H_4O_3$
Concentration	≥99% (typical reagent-grade purity — to be confirmed by the supplier's specification)
Clp index no	607-009-00-4

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][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][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).

WORKING DRAFT 工作草案

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. [12]
Advice for firefighters	Use self-contained breathing apparatus (SCBA). Full protective suit.

6. Accidental release measures

Personal precautions	Use personal protective equipment (see Section 8). Avoid breathing dust. [1][2][11]
Environmental precautions	Prevent entry into sewers, groundwater and surface water. [1][2][11]
Methods for containment and cleaning up	Collect mechanically into suitable containers. Absorption: sand, vermiculite, diatomaceous earth. Do not sweep dry (dust formation). [1][2][11]
Related sections	8; 13

7. Handling and storage

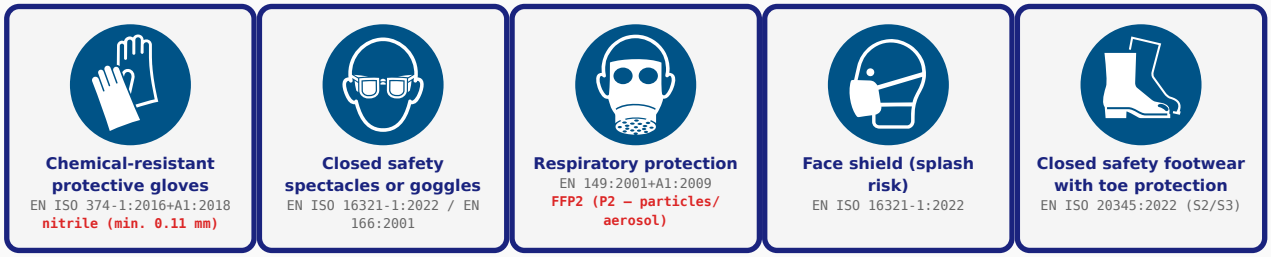
Precautions	Work in a fume hood or with adequate ventilation. No eating, drinking or smoking in the work area. [1][2][11]
Storage temperature	Store at room temperature (15-25°C) or as indicated on the label. [1][2][11]
Humidity	Store in a dry place (<60% RH). [1][2][11]
Light	Protect from direct sunlight. [1][2][11]
Incompatible materials	Strong oxidizers. [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
nitrile (min. 0.11 mm)

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

Respiratory protection
EN 149:2001+A1:2009
FFP2 (P2 — particles/ aerosol)

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	Solid	
Colour	No data available.	

WORKING DRAFT 工作稿

Property (item 9.1)	Value	Source
Odour	No data available.	
pH (1% aqueous solution)	Not applicable	
Melting point	130.8°C [8]	
Boiling point	284.1°C [8]	
Flash point	Not applicable (REACH 9.1(h))	
Flammability	No data available.	
Lower and upper explosion limit	Not applicable (REACH 9.1(g))	
Density (20°C)	1.529 g/cm³ [7]	
Vapour pressure	No data available.	
Relative vapour density	Not applicable (REACH 9.1(q))	
Kinematic viscosity	Not applicable (REACH 9.1(l))	
Auto-ignition temperature	No data available.	
Decomposition temperature	Not applicable	
Rozpuszcz. w wodzie	6 g/L, 25°C [7]	
Particle characteristics	The particle size distribution has not been determined for this commercial form — required under Annex II 9.1(r); to be completed from the supplier's specification.	
Partition coefficient n-octanol/water (log value)	1.3 [7]	
Molar mass	148.11 g/mol [7]	
Molecular formula	$C_8H_4O_3$ [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 800–1600 mg/kg; 1530 mg/kg; 4020 mg/kg (rat, oral) [7]
LD50 (dermal)	No data available.
LC50 (inhalation)	LC50 >210 mg/L (1 h) (rat) [7]
Skin irritation	Category 2 — skin irritation.
Eye irritation	Category 1 — serious eye damage.

WORKING DRAFT 工作草稿

Sensitisation	Skin, Category 1 (H317): May cause an allergic skin reaction. Respiratory tract, Category 1 (H334): May cause allergy or asthma symptoms or breathing difficulties if inhaled. [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 (H335): May cause respiratory irritation. [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]

12. Ecological information

Aquatic toxicity	EC_{50} (algae): 0.147 mg/L (Raphidocelis subcapitata, 96 h) [16]
Persistence / biodegradability	No data available.
Bioaccumulative potential	log Kow = 1.3 [7]. 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) zawierajace substancje niebezpieczne. EWC code verification required. [10]
Packaging	Cleaned packaging may be recycled. Contaminated packaging must be treated as hazardous waste.

14. Transport information

UN number	UN 2214 [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

WORKING DRAFT 工作草稿

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)

Hai-Zhe Ji, Xian-Chao Meng, Hong-Kun Zhao. (Solid + Liquid) Equilibrium of (4-Chloro-2-benzofuran-1,3-dione + 5-Chloro-2-benzofuran-1,3-dione). Journal of Chemical & Engineering Data (2009). DOI: 10.1021/je9008206

Rong-Rong Li, De-Man Han, Fu-You Pan et al.. Solid–Liquid Equilibria of Ternary 4-Nitro-2-benzofuran-1,3-dione + 5-Nitro-2-benzofuran-1,3-dione + 2-Propanone at 283.15 K and 323.15 K. Journal of Chemical & Engineering Data (2013). DOI: 10.1021/je301194e

Humaira Yasmeen Gondal, Muhammad Ali, Alain Krief et al.. 3,6-Dimethyl-o-phenylenedimethanol. Acta Crystallographica Section E (2010). DOI: 10.1107/S1600536809053513

Basketter DA, Kimber I. Phthalic anhydride: Illustrating a conundrum in chemical allergy.. Journal of immunotoxicology (2016). DOI: 10.1080/1547691X.2016.1177149

Lee YS, Jeon SH, Ham HJ et al.. Improved Anti-Inflammatory Effects of Liposomal Astaxanthin on a Phthalic Anhydride-Induced Atopic Dermatitis Model.. Frontiers in immunology (2020). DOI: 10.3389/fimmu.2020.565285

Full text of H statements

H302	Harmful if swallowed
H335	May cause respiratory irritation
H315	Causes skin irritation
H318	Causes serious eye damage
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled
H317	May cause an allergic skin reaction

Full text of P statements

P233	Keep container tightly closed
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
P272	Contaminated work clothing should not be allowed out of the workplace
P280	Wear protective gloves/protective clothing/eye protection/face protection
P284	Wear respiratory 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
P310	Immediately call a POISON CENTER or doctor/physician
P312	Call a POISON CENTER or doctor/physician if you feel unwell
P321	Specific treatment

WORKING DRAFT · 工作稿

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
P342+P311	If experiencing respiratory symptoms: Call a POISON CENTER or doctor/ physician
P362+P364	Take off contaminated clothing
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

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 (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/6811

WORKING DRAFT · 工作稿

[8] NIST. Chemistry WebBook, SRD 69. National Institute of Standards and Technology. URL: https://webbook.nist.gov/cgi/cbook.cgi?ID=85-44-9

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

[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

[11] 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

[12] Urben, 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

[15] 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

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

[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: 2026-09-23.

External links

NIST: https://webbook.nist.gov/cgi/cbook.cgi?ID=85-44-9

Wikidata: https://www.wikidata.org/wiki/Q410882

ChEMBL: https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL1371297

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: 23.09.2026 | Document version: 1

WORKING DRAFT 工作草稿