SAFETY DATA SHEET (SDS)

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

Date: 18.10.2026 | Version: 5 | EN

Methyl 4-(cyanomethyl)benzoate

methyl 4-(cyanomethyl)benzoate

CAS 76469-88-0

$C_{10}H_9NO_2$ | EC 616-338-2

MOLAR MASS	LOGP
175.18	2

TPSA: 50.1 Å²

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HAZARD CLASSIFICATION (GHS / CLP)



Warning

H302 | H312 | H315 | H319 | H332 | H412

Classification from aggregated ECHA C&L notifications (PubChem PUG-View); notifier consensus <75% — protective approach (all reported hazards). Requires 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	Methyl 4-(cyanomethyl)benzoate
1.1 IUPAC name	methyl 4-(cyanomethyl)benzoate
1.1 CAS number	76469-88-0
1.1 EC number	616-338-2
1.1 PubChem CID	848548
1.1 InChIKey	XRZGMNGGCZTNGE-UHFFFAOYSA-N
1.1 SMILES	COC(=O)C1=CC=C(C=C1)CC#N
1.1 Molecular formula	$C_{10}H_9NO_2$ [7]
1.1 Molar mass	175.18 g/mol [7]
1.1 Exact mass	175.0633 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]

H302	Harmful if swallowed
H312	Harmful in contact with skin
H315	Causes skin irritation
H319	Causes serious eye irritation
H332	Harmful if inhaled
H412	Harmful to aquatic life with long lasting effects

Precautionary statements (P) [3][4]

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
P273	Avoid release to the environment
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
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
P312	Call a POISON CENTER or doctor/physician if you feel unwell
P330	Rinse mouth
P332+P313	If skin irritation occurs: Get medical advice/attention
P337+P313	If eye irritation persists: Get medical advice/attention
P391	Collect spillage
P501	Dispose of contents/container to an approved waste collection point

Classification from aggregated ECHA C&L notifications (PubChem PUG-View); notifier consensus <75% — protective approach (all reported hazards). Requires verification against the official source (ECHA C&L / manufacturer's data sheet).

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3. Composition/information on ingredients

Substance type	pure substance
CAS Number	76469-88-0
EC number	616-338-2
Molecular formula	$C_{10}H_9NO_2$
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. 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). Call a physician immediately. [1][2][11]

Eye contact

Rinse eyes with running water (min. 15 minutes). Remove contact lenses if possible. If irritation persists — consult an ophthalmologist. [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. Emergency number: 112 (EU-wide). Contact the poison centre designated in your country (CLP Art. 45). [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: 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, NOx. [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/vapours. [1][2][11]
Environmental precautions	Prevent entry into sewers, groundwater and surface water. [1][2][11]
Methods for containment and cleaning up	Absorb with inert material (sand, vermiculite, diatomaceous earth) and collect into sealed, labelled containers. Do not release into drains. [1][2][11]
Related sections	8; 13

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7. Handling and storage

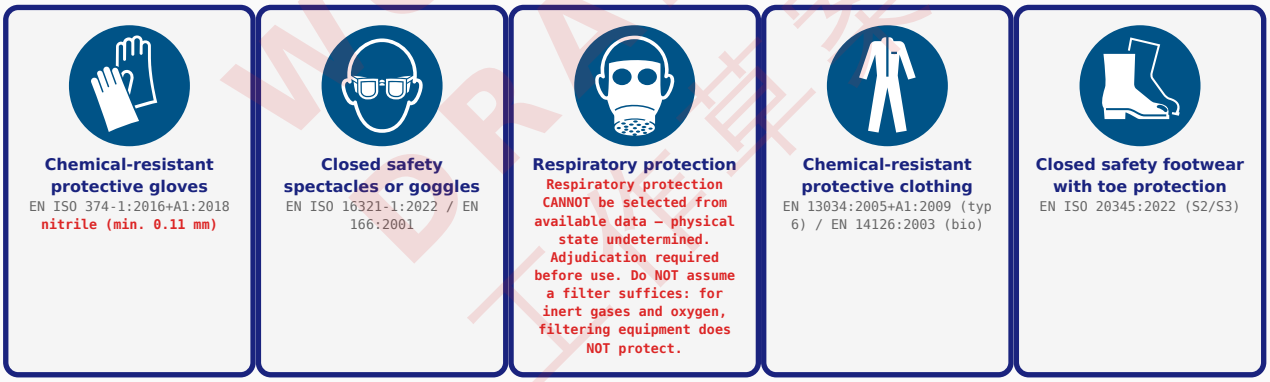
Precautions	Work in a fume hood or with adequate ventilation. No eating, drinking or smoking in the work area. [1][2][11]
Storage temperature	Store at room temperature (15-25°C) or as indicated on the label. [1][2][11]
Humidity	Store in a dry place (<60% RH). [1][2][11]
Light	Protect from direct sunlight. [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
Respiratory protection CANNOT be selected from available data — physical state undetermined. Adjudication required before use. Do NOT assume a filter suffices: for inert gases and oxygen, filtering equipment does NOT protect.

Chemical-resistant protective clothing
EN 13034:2005+A1:2009 (typ 6) / EN 14126:2003 (bio)

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	No data available.	
Colour	No data available.	
Odour	No data available.	
pH (1% aqueous solution)	No data available.	
Melting point	No data available.	
Boiling point	No data available.	
Flash point	No data available.	
Flammability	No data available.	
Lower and upper explosion limit	No data available.	
Density (20°C)	No data available.	
Vapour pressure	No data available.	

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Property (item 9.1)	Value	Source
Relative vapour density	No data available.	
Kinematic viscosity	No data available.	
Auto-ignition temperature	No data available.	
Decomposition temperature	Not applicable	
Water solubility	No data available.	
Particle characteristics	No data available.	
Partition coefficient n-octanol/water (log value)	2 [8]	
Molar mass	175.18 g/mol [7] ✓86%	*PubChem*
Molecular formula	$C_{10}H_9NO_2$ [7] ✓86%	*PubChem*
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, NOx.

11. Toxicological information

LD50 (oral)	No data available.
LD50 (dermal)	No data available.
LC50 (inhalation)	No data available.
Skin irritation	Category 2 — skin irritation.
Eye irritation	Category 2 — eye irritation.
Sensitisation	No data available.
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	No data available.
STOT — repeated exposure	No data available.
Aspiration hazard	No data available.

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12. Ecological information

Aquatic toxicity	Classification per ECHA C&L notifications (self-classification, Art. 4(3)): H412 — Harmful to aquatic life with long lasting effects (Aquatic Chronic 3). Numerical LC_{50}/EC_{50} data unverified in the available dataset — do not assume absence of toxicity.
Persistence / biodegradability	No data available.
Bioaccumulative potential	log Kow = 2 [8]. 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 (e.g. chemical reagents) containing hazardous substances. Verification of the EWC code required. [10]
Packaging	Cleaned packaging may be recycled. Contaminated packaging must be treated as hazardous waste.

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14. Transport information

UN number	VERIFICATION REQUIRED — no verified UN assignment.
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	Transport classification not verified. Do not assume the absence of restrictions — check ADR/IMDG/IATA before shipping.

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: supplier self-classification under Art. 4(3) CLP — no harmonised entry in Annex VI.Entries with an entry-into-force date after 17.10.2026 were omitted as future (not yet applicable).

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

Scientific citations (5)

Manapragada V. Rathnam, Sharad Mankumare, M. S. S. Kumar. *Density, Viscosity, and Speed of Sound of (Methyl Benzoate + Cyclohexane), (Methyl Benzoate + n-Hexane), (Methyl Benzoate + Heptane), and (Methyl Benzoate + Octane) at Temperatures of (303.15, 308.15, and 313.15) K*. Journal of Chemical & Engineering Data (2009). DOI: 10.1021/je9006597

Methyl Benzoate. Dictionary of Toxicology (2024). DOI: 10.1007/978-981-99-9283-6_1700

SHUJIRO GOYA, AKIRA TAKADATE, TOSHIAKI TANAKA et al.. *Synthesis of 6-and 7-Substituted 3-Aminoisocarbostyril Derivatives. I. Reactions of Methyl (2-Cyanomethyl) benzoate Derivatives with Amines*. YAKUGAKU ZASSHI (1980). DOI: 10.1248/yakushi1947.100.8_819

Methyl Benzoate. DOI: 10.31003/fcc_f101358_02_01

S. GOYA, A. TAKADATE, T. TANAKA et al.. *ChemInform Abstract: SYNTHESIS OF 6- AND 7-SUBSTITUTED 3-AMINOISOCARBOSTYRIL DERIVATIVES. I. REACTIONS OF METHYL (2-CYANOMETHYL)BENZOATE DERIVATIVES WITH AMINES*. Chemischer Informationsdienst (1981). DOI: 10.1002/chin.198108229

Full text of H statements

H302	Harmful if swallowed
H312	Harmful in contact with skin
H315	Causes skin irritation
H319	Causes serious eye irritation
H332	Harmful if inhaled
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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
P271	Use only outdoors or in a well-ventilated area
P273	Avoid release to the environment
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
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
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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%

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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

v5 (17.10.2026)	Based on supplier self-classification (ECHA C&L notifications; no harmonised entry in Annex VI).

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: 2026-10-17.

[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: 2026-10-17.

[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: 2026-10-17.

[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: 2026-10-17.

[5] ISO. ISO 7010:2019 — Graphical symbols. Safety signs. URL: https://www.iso.org/standard/72424.html Accessed: 2026-10-17.

[6] ISO. ISO 3864-1:2011 — Safety colours and safety signs. URL: https://www.iso.org/standard/51021.html Accessed: 2026-10-17.

[7] PubChem. National Center for Biotechnology Information (NIH/NLM), chemical compound database. URL: https://pubchem.ncbi.nlm.nih.gov/compound/848548

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

[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

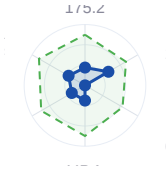
[15] European Parliament and Council. Regulation (EC) No 1907/2006 (REACH), Annex XIII — Criteria for the identification of PBT and vPvB substances. OJ EU L 396/2006 (consolidated). URL: https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:02006R1907-20140410

[16] 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: 2026-10-17.

External links

NIST: https://webbook.nist.gov/cgi/cbook.cgi?ID=76469-88-0

ADMET / Drug-likeness



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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Generator: Document generated automatically from supplier self-classification (ECHA C&L notifications) and public physicochemical databases.
Author: www.MolGod.org — platform for automated safety data sheets (SDS).
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