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

Walina

(2S)-2-amino-3-methylbutanoic acid

CAS 72-18-4

$C_5H_{11}NO_2$ | EC 200-773-6

易 普 化 工
EAPEARL CHEM

MOLAR MASS	LOGP
117.15	-2.3

HAZARD CLASSIFICATION (GHS / CLP)

CLP classification not established — no harmonised entry (Annex VI), and the provenance of the self-classification has not been established. Verification in the ECHA C&L inventory / the manufacturer's safety data sheet is required. Do NOT assume the absence of hazard.

1. Identification of the substance/mixture and of the company/undertaking

1.1 Substance name	Walina
1.1 IUPAC name	(2S)-2-amino-3-methylbutanoic acid
1.1 CAS number	72-18-4
1.1 EC number	200-773-6
1.1 PubChem CID	6287
1.1 InChIKey	KZSNJWFQEVHDMF-BYPYZUCNSA-N
1.1 SMILES	CC(C)[C@@H](C(=O)O)N
1.1 Molecular formula	$C_5H_{11}NO_2$ [7]
1.1 Molar mass	117.15 g/mol [7]
1.1 Exact mass	117.0790 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

CLP classification not established — no harmonised entry (Annex VI), and the provenance of the self-classification has not been established. Verification in the ECHA C&L inventory / the manufacturer's safety data sheet is required. Do NOT assume the absence of hazard.

3. Composition/information on ingredients

Substance type	pure substance
CAS Number	72-18-4
EC number	200-773-6
Molecular formula	$C_5H_{11}NO_2$
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]

Skin contact

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

Eye contact

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

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]

Symptoms and effects

No specific symptoms described in the literature. [1][2]

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.
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]
Environmental precautions	Prevent entry into sewers, groundwater and surface water. [1][2]
Methods for containment and cleaning up	Collect mechanically into suitable containers. Absorption: sand, vermiculite, diatomaceous earth. Do not sweep dry (dust formation). [1][2]
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]
Storage temperature	Store at room temperature (15-25°C) or as indicated on the label. [1][2]
Humidity	Store in a dry place (<60% RH). [1][2]
Light	Protect from direct sunlight. [1][2]

WORKING DRAFT 工作草案

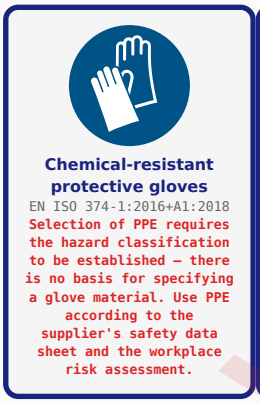
Incompatible materials	Strong oxidizers, strong bases, Base metals (hydrogen evolution).

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)



Chemical-resistant protective gloves

EN ISO 374-1:2016+A1:2018

Selection of PPE requires the hazard classification to be established — there is no basis for specifying a glove material. Use PPE according to the supplier's safety data sheet and the workplace risk assessment.



Closed safety spectacles or goggles

EN ISO 16321-1:2022 / EN 166:2001



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.	
Odour	No data available.	
pH (1% aqueous solution)	No data available.	
Melting point	315°C [7]	
Boiling point	No data available.	
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)	1.23 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	No data available.	
Rozpuszcz. w wodzie	58.5 g/L, 25°C [7]	

WORKING DRAFT 工作草稿

Property (item 9.1)	Value	Source
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)	-2.3 [7]	
Molar mass	117.15 g/mol [7]	
Molecular formula	$C_5H_{11}NO_2$ [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, strong bases, Base metals (hydrogen evolution).
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	No data available.
Eye irritation	No data available.
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.

WORKING DRAFT · 工作稿

12. Ecological information

Aquatic toxicity	No data available.
Persistence / biodegradability	No data available.
Bioaccumulative potential	log Kow = -2.3 [7]. Low bioaccumulation potential (log Kow < 4.5 — PBT/vPvB screening criterion per ECHA Guidance R.11). [9][10]
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)	The waste code (EWC) cannot be determined without a hazard classification — the provenance of the classification has not been established. Do NOT assume either hazardousness (16 05 06*) or the absence thereof (16 05 09); determine it after verifying the classification in ECHA. [8]
Packaging	Cleaned packaging may be recycled. Contaminated packaging must be handled in accordance with the waste classification (see the EWC code above); where no classification has been established, do not assume the absence of hazard.

14. Transport information

UN number	VERIFICATION REQUIRED — no verified UN assignment.
Environmental hazard	Environmental hazard for transport: not verified. Classification provenance undetermined — do NOT assume absence of environmental hazard or that marine pollutant marking is not required; verify against CLP Annex VI, Section 12 and ADR 2.2.9 / IMDG criteria 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: provenance not recorded — requires verification in ECHA.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)

Amalendu Pal, Nalin Chauhan. Thermodynamic Study of Some Amino Acids, 2-Aminopropanoic Acid, 2-Amino-3-methylbutanoic Acid, 2-Amino-4-methylpentanoic Acid, and 2-Amino-3-phenylpropanoic Acid in Aqueous Saccharide Solutions at Different Temperatures: Volumetric and Ultrasonic Study. Journal of Chemical & Engineering Data (2011). DOI: 10.1021/je100857s

WORKING DRAFT · 工作草案

Zhenning Yan, Yang Zhao, Ronghua Xing et al.. Volumetric and Conductometric Behavior at T = 298.15 K of 2-[(2-Aminoacetyl)amino]acetic Acid, 2-[(2-Aminoacetyl)amino]-3-methylbutanoic Acid, and (2S)-2-[(2-Aminoacetyl)amino]-4-methylpentanoic Acid with Sodium Hexanoate. Journal of Chemical & Engineering Data (2009). DOI: 10.1021/je900449q

Maria Annunziata M. Capozzi, Cosimo Cardellicchio. (S,S)-2-(((Hydroxynaphth-1-yl)(4′-nitrophenyl)methyl)amino)-3-methylbutanoic Acid Methyl Ester. Molbank (2022). DOI: 10.3390/m1528

Jiarui Lu, Yuyang Wang, Yizhe Zhang et al.. SimpleDesign: A Joint Model for Protein Sequence and Structure Codesign. arXiv (2609.03377v1) (2026).

Boheng Guan, Xuyu Liu. (R)-2-Amino-3-mercapto-3-methylbutanoic Acid. Encyclopedia of Reagents for Organic Synthesis (2026). DOI: 10.1002/047084289x.rn02173

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)	Classification provenance not recorded in the canon — verify the source in ECHA (Annex VI / C&L).

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/6287

[8] 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

[9] 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

[10] 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

WORKING DRAFT · 工作草稿

[11] 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=72-18-4

Wikidata: https://www.wikidata.org/wiki/Q483752

ChEMBL: https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL43068

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 classification of unrecorded provenance (to be verified in ECHA) 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