# SAFETY DATA SHEET (SDS)

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

Date: 18.10.2026 | Version: 4 | EN

## L-Alanine, N-((S)-(2,3,4,5,6-pentafluorophenoxy)phenoxyphosphinyl)-, 1-methylethyl ester

*propan-2-yl (2S)-2-[[(2,3,4,5,6-pentafluorophenoxy)-phenoxyphosphoryl]amino]propanoate*

**CAS 1334513-02-8**

$C_{18}H_{17}F_5NO_5P$ | EC 695-076-0

| MOLAR MASS | LOGP |
|---|---|
| 453.30 | 4.5 |

TPSA: 73.9 Å²

### 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** | L-Alanine, N-((S)-(2,3,4,5,6-pentafluorophenoxy)phenoxyphosphinyl)-, 1-methylethyl ester |
| **1.1 IUPAC name** | propan-2-yl (2S)-2-[[(2,3,4,5,6-pentafluorophenoxy)-phenoxyphosphoryl]amino]propanoate |
| **1.1 CAS number** | 1334513-02-8 |
| **1.1 EC number** | 695-076-0 |
| **1.1 PubChem CID** | 49820457 |
| **1.1 InChIKey** | MIILDBHEJQLACD-KPORQTCDSA-N |
| **1.1 SMILES** | C[C@@H](C(=O)OC(C)C)NP(=O)(OC1=CC=CC=C1)OC2=C(C(=C(C(=C2F)F)F)F)F |
| **1.1 Molecular formula** | $C_{18}H_{17}F_5NO_5P$ [7] |
| **1.1 Molar mass** | 453.3 g/mol [7] |
| **1.1 Exact mass** | 453.0765 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

**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** | 1334513-02-8 |
| **EC number** | 695-076-0 |
| **Molecular formula** | $C_{18}H_{17}F_5NO_5P$ |
| **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. Emergency number: 112 (EU-wide). Contact the poison centre designated in your country (CLP Art. 45). [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, HF, P2O5. |
| **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] |
| **Environmental precautions** | Prevent entry into sewers, groundwater and surface water. [1][2] |
| **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] |
| **Related sections** | 8; 13 |

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## 7. Handling and storage

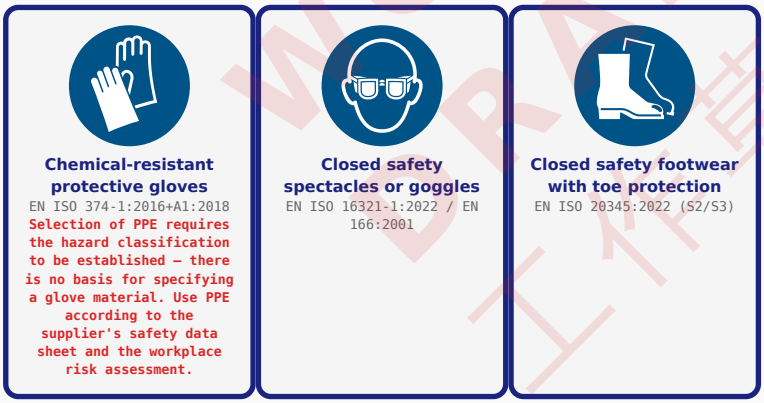
| | |
|---|---|
| **Precautions** | Work in a fume hood or with adequate ventilation. No eating, drinking or smoking in the work area. [1][2] |
| **Storage temperature** | Store at room temperature (15-25°C) or as indicated on the label. [1][2] |
| **Humidity** | Store in a dry place (<60% RH). [1][2]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

## 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** | 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. | |

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| Property (item 9.1) | Value | Source |
|---|---|---|
| **Vapour pressure** | No data available. | |
| **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)** | 4.5 [8] | |
| **Molar mass** | 453.3 g/mol [7] ✓86% | *PubChem* |
| **Molecular formula** | $C_{18}H_{17}F_5NO_5P$ [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, HF, P2O5. |

## 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. |

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## 12. Ecological information

| | |
|---|---|
| **Aquatic toxicity** | No data available. |
| **Persistence / biodegradability** | No data available. |
| **Bioaccumulative potential** | log Kow = 4.5 [8]. Elevated bioaccumulation potential (log Kow ≥ 4.5 — PBT/vPvB screening threshold per ECHA R.11); a definitive assessment requires the bioconcentration factor BCF (REACH Annex XIII: B if BCF > 2000). [10][11] |
| **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. [9] |
| **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 after 17.10.2026 were omitted as future (not yet applicable).

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

### Abbreviations

| | |
|---|---|
| **ADR** | European Agreement concerning the International Carriage of Dangerous Goods by Road |
| **ATE** | Acute Toxicity Estimate |

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| | |
|---|---|
| **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

| | |
|---|---|
| **v4 (17.10.2026)** | 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: 2026-10-17.

[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/53476763

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

[9] 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

[10] 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

[11] 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

[12] 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=1334513-02-8

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**ADMET / Drug-likeness**




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