# 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

## Phenylethyl isovalerate

*2-phenylethyl 3-methylbutanoate*

**CAS 140-26-1**

$C_{13}H_{18}O_2$ | EC 205-406-3

| MOLAR MASS | LOGP |
|---|---|
| 206.28 | 3.6 |
| **TPSA** | **T. WRZ.** |
| 26.3 Å² | 263.00°C |

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## HAZARD CLASSIFICATION (GHS / CLP)



**Warning**

H411

*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** | Phenylethyl isovalerate |
| **1.1 IUPAC name** | 2-phenylethyl 3-methylbutanoate |
| **1.1 CAS number** | 140-26-1 |
| **1.1 EC number** | 205-406-3 |
| **1.1 PubChem CID** | 8792 |
| **1.1 InChIKey** | JIMGVOCOYZFDKB-UHFFFAOYSA-N |
| **1.1 SMILES** | CC(C)CC(=O)OCCC1=CC=CC=C1 |
| **1.1 Molecular formula** | $C_{13}H_{18}O_2$ [7] |
| **1.1 Molar mass** | 206.28 g/mol [7] |
| **1.1 Exact mass** | 206.1307 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:**



**Warning**

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

| | |
|---|---|
| **H411** | Toxic to aquatic life with long lasting effects |

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

| | |
|---|---|
| **P273** | Avoid release to the environment |
| **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** | 140-26-1 |
| **EC number** | 205-406-3 |
| **Molecular formula** | $C_{13}H_{18}O_2$ |
| **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. 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. 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

No specific symptoms described in the literature. [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. [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 |

## 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] |

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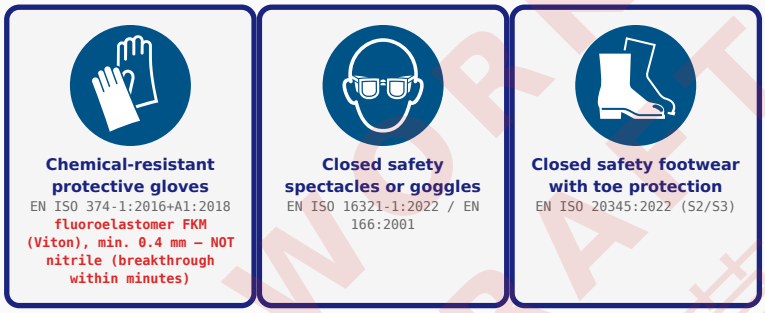
| | |
|---|---|
| **Humidity** | Store in a dry place (<60% RH). [1][2][11] |
| **Light** | Protect from direct sunlight. [1][2][11] |
| **Incompatible materials** | Strong oxidizers. [12] |

## 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
fluoroelastomer FKM (Viton), min. 0.4 mm — NOT nitrile (breakthrough within minutes)

**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** | 263.00°C (experimental data) [7] | *PubChem (experimental data)* |
| **Flash point** | No data available. | |
| **Flammability** | No data available. | |
| **Lower and upper explosion limit** | No data available. | |
| **Density (20°C)** | 0.974 g/cm³ [7] ✓86% | *source consensus, PubChem (experimental data)* |
| **Vapour pressure** | No data available. | |
| **Relative vapour density** | No data available. | |
| **Kinematic viscosity** | No data available. | |
| **Refractive index $nD^{20}$** | 1.482 (experimental data) [7] | |
| **Auto-ignition temperature** | No data available. | |
| **Decomposition temperature** | Not applicable | |

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| Property (item 9.1) | Value | Source |
|---|---|---|
| **Water solubility** | No data available. | |
| **Particle characteristics** | No data available. | |
| **Partition coefficient n-octanol/water (log value)** | 3.6 [8] | |
| **Molar mass** | 206.28 g/mol [7] ✓86% | *PubChem* |
| **Molecular formula** | $C_{13}H_{18}O_2$ [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. |

## 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** | Classification per ECHA C&L notifications (self-classification, Art. 4(3)): H411 — Toxic to aquatic life with long lasting effects (Aquatic Chronic 2). 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 = 3.6 [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. |

## 14. Transport information

| | |
|---|---|
| **UN number** | VERIFICATION REQUIRED — no verified UN assignment. |
| **Environmental hazard** | CLP classification (H411) indicates aquatic environmental hazard — marine pollutant marking may be required; confirm per ADR 2.2.9 / IMDG criteria [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** | Transport classification not verified. Do not assume the absence of restrictions — check ADR/IMDG/IATA before shipping. |
| **Environmentally hazardous (mark: fish and tree)** | Yes |

## 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 (1)

Api AM, Belsito D, Botelho D et al.. *RIFM fragrance ingredient safety assessment phenethyl isovalerate, CAS Registry Number 140-26-1.*. Food and chemical toxicology : an international journal published for the British Industrial Biological Research Association (2018). DOI: 10.1016/j.fct.2018.01.006

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## Full text of H statements

| | |
|---|---|
| **H411** | Toxic to aquatic life with long lasting effects |

## Full text of P statements

| | |
|---|---|
| **P273** | Avoid release to the environment |
| **P391** | Collect spillage |
| **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

| | |
|---|---|
| **v4 (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/8792

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


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[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

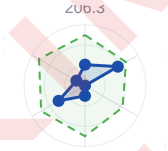
[15] European Parliament and Council. Regulation (EC) No 1907/2006 (REACH), Annex XIII — Criteria for the identification of PBT and vPvB substances. OJ EU L 396/2006 (consolidated). URL: https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:02006R1907-20140410

[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=140-26-1

**ADMET / Drug-likeness**




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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).
Issue date: 18.10.2026 | Document version: 4