SAFETY DATA SHEET (SDS)

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

Date: 21.10.2026 | Version: 6 | EN

2-Ethylhexanoic Acid

2-ethylhexanoic acid

CAS 149-57-5

$C_8H_{16}O_2$ | EC 205-743-6

MOLAR MASS	LOGP
144.21	2.6

HAZARD CLASSIFICATION (GHS / CLP)



Warning

H361

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	2-Ethylhexanoic Acid
1.1 IUPAC name	2-ethylhexanoic acid
1.1 CAS number	149-57-5
1.1 EC number	205-743-6
1.1 PubChem CID	8697
1.1 InChIKey	OBETXYAYXDNJHR-UHFFFAOYSA-N
1.1 SMILES	CCCCC(CC)C(=O)O
1.1 Molecular formula	$C_8H_{16}O_2$ [7]
1.1 Molar mass	144.21 g/mol [7]
1.1 Exact mass	144.1150 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]

H361	Suspected of damaging fertility or the unborn child

Precautionary statements (P) [3][4]

P201	Obtain special instructions before use
P202	Do not handle until all safety precautions have been read and understood
P280	Wear protective gloves/protective clothing/eye protection/face protection
P308+P313	IF exposed or concerned: Get medical advice/attention
P405	Store locked up
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).

WORKING DRAFT · 工作草案

3. Composition/information on ingredients

Substance type	pure substance
CAS Number	149-57-5
EC number	205-743-6
Molecular formula	$C_8H_{16}O_2$
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][12]

Skin contact

Remove contaminated clothing. Rinse skin with soap and water (min. 15 minutes). [1][2][12]

Eye contact

Rinse eyes with running water (min. 15 minutes). Remove contact lenses if possible. If irritation persists — consult an ophthalmologist. [1][2][12]

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][12]

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. [13]
Advice for firefighters	Use self-contained breathing apparatus (SCBA). Full protective suit.
Flash Point	114°C [7]
Auto-ignition temperature	370.6°C [7]

6. Accidental release measures

Personal precautions	Use personal protective equipment (see Section 8). Avoid breathing vapours. [1][2][12]
Environmental precautions	Prevent entry into sewers, groundwater and surface water. [1][2][12]
Methods for containment and cleaning up	Contain the spill with a barrier. Absorb with inert material (sand, vermiculite, diatomaceous earth). Collect into sealed, labelled containers. Do not release into drains. [1][2][12]
Related sections	8; 13

WORKING DRAFT 工作草案

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][12]
Storage temperature	Store at room temperature (15-25°C) or as indicated on the label. [1][2][12]
Humidity	Store in a dry place (<60% RH). [1][2][12]
Light	Protect from direct sunlight. [1][2][12]
Incompatible materials	Strong oxidizers, strong bases, Base metals (hydrogen evolution). [13]

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][16]



9. Physical and chemical properties

Property (item 9.1)	Value	Source
Physical state	Liquid	
Colour	Clear liquid [7]	
Odour	Mild odor [7]	
pH (1% aqueous solution)	No data available.	
Melting point	-59.00°C (experimental data) [7]	
Boiling point	228.0673°C [8] [7]	
Flash point	114°C (experimental data) [7]	
Flammability	No data available.	
Lower and upper explosion limit	No data available.	
Density (20°C)	0.903 g/cm³ (experimental data) [7]	
Vapour pressure	0.004 kPa (0.03 mmHg, 20°C) (experimental data) [7]	
Relative vapour density	4.98 [20]	
Dynamic viscosity	7.8 mPa·s [7]	

WORKING DRAFT 工作草稿

Property (item 9.1)	Value	Source
Kinematic viscosity	No data available.	
Refractive index nD^{20}	1.4241 (experimental data) [7]	
Auto-ignition temperature	370.6°C (experimental data) [7]	
Decomposition temperature	Not applicable	
Water solubility	2 g/L, 20°C [7]	
Particle characteristics	Not applicable (REACH 9.1(r))	
Partition coefficient n-octanol/water (log value)	2.6 [9]	
Molar mass	144.21 g/mol [7]	
Molecular formula	$C_8H_{16}O_2$ [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.

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	Classification from aggregated ECHA C&L notifications (non-harmonised) — requires verification; no entry in Annex VI to CLP.
STOT — single exposure	No data available.
STOT — repeated exposure	No data available.
Aspiration hazard	No data available.

WORKING DRAFT 工作草案

12. Ecological information

Aquatic toxicity	EC_{50} (Daphnia): 106 mg/L (Daphnia magna, 48 h) [19]
Persistence / biodegradability	No data available.
Bioaccumulative potential	log Kow = 2.6 [9]. Low bioaccumulation potential (log Kow < 4.5 — PBT/vPvB screening criterion per ECHA Guidance R.11). [17][18]
Mobility in soil	No data available.
PBT/vPvB assessment	Insufficient data to assess PBT/vPvB.
Endocrine disrupting properties	Reported endocrine effects in aquatic organisms (ecotoxicological data, US EPA ECOTOX; not a regulatory ED classification under 2018/605). [19]

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. [11]
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	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 21.10.2026 were omitted as future (not yet applicable).

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

Scientific citations (7)

Juberg DR, David RM, Katz GV et al.. *2-Ethylhexanoic acid: subchronic oral toxicity studies in the rat and mouse.*. Food and chemical toxicology : an international journal published for the British Industrial Biological Research Association (1998). DOI: 10.1016/s0278-6915(97)00168-3

Obringer C, Lester C, Karb M et al.. *Impact of chemical structure on the in vitro hydrolysis of fatty esters of 2-ethylhexanoic acid or 2-ethylhexanol and extrapolation to the in vivo situation.*. Regulatory toxicology and pharmacology : RTP (2023). DOI: 10.1016/j.yrtph.2022.105315

Bui LM, Taubeneck MW, Commisso JF et al.. *Altered zinc metabolism contributes to the developmental toxicity of 2-ethylhexanoic acid, 2-ethylhexanol and valproic acid.*. Toxicology (1998). DOI: 10.1016/s0300-483x(97)00171-6

WORKING DRAFT · 工作草稿

Pennanen S, Manninen A. *Distribution of 2-ethylhexanoic acid in mice and rats after an intraperitoneal injection.*. Pharmacology & toxicology (1991). DOI: 10.1111/j.1600-0773.1991.tb01208.x

French KJ, Strickler MD, Rock DA et al.. *Benign synthesis of 2-ethylhexanoic acid by cytochrome P450cam: enzymatic, crystallographic, and theoretical studies.*. Biochemistry (2001). DOI: 10.1021/bi010063+

Full text of H statements

H361	Suspected of damaging fertility or the unborn child

Full text of P statements

P201	Obtain special instructions before use
P202	Do not handle until all safety precautions have been read and understood
P280	Wear protective gloves/protective clothing/eye protection/face protection
P308+P313	IF exposed or concerned: Get medical advice/attention
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

v6 (21.10.2026)	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: 2026-10-21.

WORKING DRAFT · 工作草稿

[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: 2026-10-21.

[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: 2026-10-21.

[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: 2026-10-21.

[5] ISO. ISO 7010:2019 — Graphical symbols. Safety signs. URL: https://www.iso.org/standard/72424.html Accessed: 2026-10-21.

[6] ISO. ISO 3864-1:2011 — Safety colours and safety signs. URL: https://www.iso.org/standard/51021.html Accessed: 2026-10-21.

[7] PubChem. National Center for Biotechnology Information (NIH/NLM), chemical compound database. URL: https://pubchem.ncbi.nlm.nih.gov/compound/8697

[8] NIST. Chemistry WebBook, SRD 69. National Institute of Standards and Technology. URL: https://webbook.nist.gov/cgi/cbook.cgi?ID=149-57-5

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

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

[11] 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

[12] 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

[13] Urben, P.G., ed. Bretherick's Handbook of Reactive Chemical Hazards. 8th ed. Oxford: Academic Press.

[14] Act of 26 June 1974 — Labour Code (Poland), Art. 176 § 1. Journal of Laws 2023 item 1465. URL: https://isap.sejm.gov.pl

[15] Council of Ministers of the Republic of Poland. Regulation of 3 April 2017 on the list of arduous, hazardous or health-harmful work for pregnant and breastfeeding women. Journal of Laws 2017 item 796. URL: https://isap.sejm.gov.pl/isap.nsf/DocDetails.xsp?id=WDU20170000796

[16] CEN. Personal protective equipment standards (EN ISO 374-1, EN 166, EN 149, EN 14387, EN ISO 20345). Brussels: European Committee for Standardization.

[17] 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

[18] 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

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

[20] MOL-GOD. Value obtained by calculation from the molecular formula/molecular weight (the specific quantity and its formula are indicated at the respective field). Calculated value, not an experimental measurement. URL: https://www.nist.gov/pml/atomic-weights-and-isotopic-compositions-relative-atomic-masses

[21] 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: 2026-10-21.

External links

NIST: https://webbook.nist.gov/cgi/cbook.cgi?ID=149-57-5

ChEMBL: https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL1162485

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) 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 supplier self-classification (ECHA C&L notifications) and public physicochemical databases.
Author: www.MolGod.org — platform for automated safety data sheets (SDS).
Issue date: 21.10.2026 | Document version: 6