

SAFETY DATA SHEET (SDS)

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

Date: 03.09.2026 | Version: 1 | EN

[2,2,4-trimethyl-3-(2-methylpropanoyloxy)pentyl] 2-methylpropanoate

[2,2,4-trimethyl-3-(2-methylpropanoyloxy)pentyl] 2-methylpropanoate

CAS 6846-50-0

 $C_{16}H_{30}O_4$ MOLAR MASS
286.41LOGP
4.7

HAZARD CLASSIFICATION (GHS / CLP)



Warning

H401 H412

Non-harmonised classification (no entry in Annex VI to CLP) — assigned from aggregated ECHA C&L notifications; the H-statements require 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

1.1 IUPAC name

[2,2,4-trimethyl-3-(2-methylpropanoyloxy)pentyl] 2-methylpropanoate

1.1 CAS number

6846-50-0

1.1 EC number

No data

1.1 PubChem CID

23284

1.1 InChIKey

OMVSWZDEEGJJJ-UHFFFAOYSA-N

1.1 SMILES

CC(C)C(C(C)(C)COC(=O)C(C)C)OC(=O)C(C)C

1.1 Molecular formula

 $C_{16}H_{30}O_4$ ^[7]

1.1 Molar mass

286.41 g/mol ^[7]

1.1 Exact mass

286.2144 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)

2. Hazards identification

GHS:



PPE:



Warning

Hazard statements (H) ^{[3][4]}

H401	Toxic to aquatic life
H412	Harmful 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

Non-harmonised classification (no entry in Annex VI to CLP) — assigned from aggregated ECHA C&L notifications; the H-statements require verification against the official source (ECHA C&L / manufacturer's data sheet).

3. Composition/information on ingredients

Substance type	pure substance
CAS Number	6846-50-0
Molecular formula	$C_{16}H_{30}O_4$
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][10]}

Skin contact

Remove contaminated clothing. Rinse skin with soap and water (min. 15 minutes). ^{[1][2][10]}

Eye contact

Rinse eyes with running water (min. 15 minutes). Remove contact lenses if possible. If irritation persists — consult an ophthalmologist. ^{[1][2][10]}

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][10]}

Symptoms and effects

No specific symptoms described in the literature. ^[3]

Notes for physician

Requires verification

Emergency numbers: CIT Łódź: +48 42 631 47 24 (24/7) | Emergency: 112

5. Firefighting measures

Suitable extinguishing media	Adapt extinguishing media to surroundings. CO ₂ , dry powder, foam.
Unsuitable extinguishing media	No specific restrictions.
Specific hazards	Thermal decomposition products: CO, CO ₂ . ^[11]
Advice for firefighters	Use self-contained breathing apparatus (SCBA). Full protective suit.
Flash Point	121°C ^[7]
Auto-ignition temperature	424°C ^[7]

6. Accidental release measures

Personal precautions	Use personal protective equipment (see Section 8). Avoid breathing dust/vapours. ^{[1][2][10]}
Environmental precautions	Prevent entry into sewers, groundwater and surface water. ^{[1][2][10]}
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][10]}
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][10]}
Storage temperature	Store at room temperature (15-25°C) or as indicated on the label. ^{[1][2][10]}

Humidity	Store in a dry place (<60% RH). ^{[1][2][10]}
Light	Protect from direct sunlight. ^{[1][2][10]}
Incompatible materials	Strong oxidizers. ^[11]

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][12]}



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



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	380°C (experimental data) ^[7]	
Flash point	121°C (experimental data) ^[7]	
Flammability	No data available.	
Lower and upper explosion limit	No data available.	
Density (20°C)	0.94 g/cm ³ ^[7]	
Vapour pressure	No data available.	
Relative vapour density	No data available.	
Kinematic viscosity	No data available.	
Auto-ignition temperature	424°C (experimental data) ^[7]	
Decomposition temperature	Not applicable	
Rozpuszcz. w wodzie	No data available.	
Particle characteristics	No data available.	

Property (item 9.1)	Value	Source
Partition coefficient n-octanol/water (log value)	4.7 ^[8]	
Molar mass	286.41 g/mol ^[7]	
Molecular formula	C ₁₆ H ₃₀ O ₄ ^[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.
Decomposition products	Thermal decomposition products:CO, CO2.

11. Toxicological information

LD50 (oral)	LD50 >3200 mg/kg (rat, oral) ^[7]
LD50 (dermal)	No data available.
LC50 (inhalation)	LC50 >5.3 mg/L (rat) ^[7]
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.

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 = 4.7 ^[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). ^{[13][14]}
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 (np. chemical reagents) zawierające substancje niebezpieczne. EWC code verification required. ^[9]
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 03.09.2026 were omitted as future (not yet applicable).

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

Scientific citations (10)

- Yaping Wang, Min Liu, Fude Yang et al.. The associations of socioeconomic status, social activities, and loneliness with depressive symptoms in adults aged 50 years and older across 24 countries: findings from five prospective cohort studies.. The Lancet Healthy Longevity (2024). DOI: 10.1016/j.lanhl.2024.07.001
- Simiao Chen, Michael Kuhn, K. Prettnner et al.. The global economic burden of chronic obstructive pulmonary disease for 204 countries and territories in 2020–50: a health-augmented macroeconomic modelling study. Lancet Global Health (2023). DOI: 10.1016/S2214-109X(23)00217-6
- F. Knop, V. Aroda, Ruben D do Vale et al.. Oral semaglutide 50 mg taken once per day in adults with overweight or obesity (OASIS 1): a randomised, double-blind, placebo-controlled, phase 3 trial.. The Lancet (2023). DOI: 10.1016/S0140-6736(23)01185-6
- A. Wexler, S. Hasegawa. Relative Humidity-Temperature Relationships of Some Saturated Salt Solutions in the Temperature Range 0 0 to 50 0 C 1. (2011).
- Jianguo Wang, Yu Wang, Xiangyang Peng et al.. Induced Voltage of Overhead Ground Wires in 50 0-kV Single-Circuit Transmission Lines. IEEE Transactions on Power Delivery (2014). DOI: 10.1109/TPWRD.2013.2251371

Full text of H statements

H401	Toxic to aquatic life
H412	Harmful 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

v1 (03.09.2026)	Based on supplier self-classification (ECHA C&L notifications; no harmonised entry in Annex VI).
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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: 2026-09-03.
- [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: 2026-09-03.
- [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: 2026-09-03.
- [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: 2026-09-03.
- [5] ISO. ISO 7010:2019 — Graphical symbols. Safety signs. URL: <https://www.iso.org/standard/72424.html> Accessed: 2026-09-03.
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- [7] PubChem. National Center for Biotechnology Information (NIH/NLM), chemical compound database. URL: <https://pubchem.ncbi.nlm.nih.gov/compound/23284>
- [8] Rumble, J.R., ed. CRC Handbook of Chemistry and Physics. 105th ed. Boca Raton: CRC Press, 2024. URL: <https://hbcpc.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] 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
- [11] Urban, P.G., ed. Bretherick's Handbook of Reactive Chemical Hazards. 8th ed. Oxford: Academic Press.
- [12] CEN. Personal protective equipment standards (EN ISO 374-1, EN 166, EN 149, EN 14387, EN ISO 20345). Brussels: European Committee for Standardization.
- [13] 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>
- [14] 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>
- [15] 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: 2026-09-03.

External links

NIST: <https://webbook.nist.gov/cgi/cbook.cgi?ID=6846-50-0>

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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