

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

xlenol

2,3-dimethylphenol

CAS 1300-71-6

 $C_8H_{10}O$

EC 215-089-3

MOLAR MASS
122.16LOGP
2.60
(estymacja
LLM)

HAZARD CLASSIFICATION (GHS / CLP)



Danger

H311 H301 H314 H411

Hazard class scope limited to the harmonised classification (CLP Annex VI); classes outside the harmonised entry may require supplier self-classification (CLP Art. 4(3)) — verify with the supplier safety data sheet.

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

1.1 Substance name	xlenol
1.1 IUPAC name	2,3-dimethylphenol
1.1 CAS number	1300-71-6
1.1 EC number	215-089-3
1.1 PubChem CID	10687
1.1 InChIKey	QWBBPBRQALCEIZ-UHFFFAOYSA-N
1.1 SMILES	<chem>CC1=C(C(=CC=C1)O)C</chem>
1.1 Molecular formula	$C_8H_{10}O$ ^[7]
1.1 Molar mass	122.16 g/mol ^[7]
1.1 Exact mass	122.0732 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)

The number above is the Polish poison centre (CIT, Lodz, 24/7). It is NOT the poison centre designated for your country. Under Article 45 of Regulation (EC) No 1272/2008 the competent body is the centre designated in the country of placing on the market — consult it before use.

2. Hazards identification



Danger

Hazard statements (H) ^{[3][4][8]}

H311	Toxic in contact with skin
H301	Toxic if swallowed
H314	Causes severe skin burns and eye damage
H411	Toxic to aquatic life with long lasting effects

Precautionary statements (P) ^{[3][4][8]}

P260	Do not breathe dust/fume/gas/mist/vapours/spray
P264	Wash thoroughly after handling
P270	Do not eat, drink or smoke when using this product
P273	Avoid release to the environment
P280	Wear protective gloves/protective clothing/eye protection/face protection
P301+P310	IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician
P301+P330+P331	IF SWALLOWED: Rinse mouth; Do NOT induce vomiting
P302+P352	IF ON SKIN: Wash with plenty of water
P303+P361+P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing; Rinse skin with water or shower
P304+P340	IF INHALED: Remove person to fresh air and keep comfortable for breathing
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes; Remove contact lenses, if present and easy to do. Continue rinsing
P310	Immediately call a POISON CENTER or doctor/physician
P312	Call a POISON CENTER or doctor/physician if you feel unwell
P321	Specific treatment
P330	Rinse mouth
P363	Wash contaminated clothing before reuse
P391	Collect spillage
P405	Store locked up
P501	Dispose of contents/container to an approved waste collection point

3. Composition/information on ingredients

Substance type	pure substance
CAS Number	1300-71-6
EC number	215-089-3
Molecular formula	C ₈ H ₁₀ O
Concentration	≥99% (typical reagent-grade purity — to be confirmed by the supplier's specification)
Clp index no	604-006-00-X

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). Call a physician immediately. ^{[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

nausea, vomiting, diarrhoea; skin redness and irritation. ^{[3][8]}

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	-95°C ^[7]
Auto-ignition temperature	598.9°C ^[7]

6. Accidental release measures

Personal precautions	Use personal protective equipment (see Section 8). Avoid breathing vapours. ^{[1][2][10]}
Environmental precautions	Prevent entry into sewers, groundwater and surface water. ^{[1][2][10]}
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][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	 Face shield (splash risk) EN ISO 16321-1:2022	 Chemical-resistant protective clothing EN 13034:2005+A1:2009 (typ 6) / EN 14126:2003 (bio)	 Closed safety footwear with toe protection EN ISO 20345:2022 (S2/S3)
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9. Physical and chemical properties

UWAGA: Substancja może zestalać się w temperaturze poniżej 20.0°C.

Property (item 9.1)	Value	Source
Physical state	Liquid	
Colour	No data available.	
Odour	No data available.	
pH (1% aqueous solution)	No data available.	
Melting point	20°C (experimental data) ^[7]	
Boiling point	203°C (experimental data) ^[7]	
Flash point	-95°C (experimental data) ^[7]	
Flammability	No data available.	
Lower and upper explosion limit	No data available.	
Density (20°C)	1.0345 g/cm ³ ^[7]	
Vapour pressure	0.012 kPa (0.089 mmHg, 25°C) (experimental data) ^[7]	
Relative vapour density	4.22 ^[15]	

Property (item 9.1)	Value	Source
Dynamic viscosity	1.845 mPa·s ^[7]	
Kinematic viscosity	No data available.	
Refractive index n _D ²⁰	1.542 (experimental data) ^[7]	
Auto-ignition temperature	598.9°C (experimental data) ^[7]	
Decomposition temperature	Not applicable	
Rozpuszcz. w wodzie	4.57 g/L, 25°C ^[7]	
Particle characteristics	Not applicable (REACH 9.1(r))	
log K _{ow} (XLogP3)	2.6 ^[7]	
Molar mass	122.16 g/mol ^[7]	
Molecular formula	C ₈ H ₁₀ O ^[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, CO ₂ .

11. Toxicological information

LD50 (oral)	No data available.
LD50 (dermal)	No data available.
LC50 (inhalation)	No data available.
Skin irritation	Category 1 (H314) — corrosive; sub-category (1A/1B/1C) per CLP Annex VI entry. ^{[3][8]}
Eye irritation	Serious eye damage — covered by the corrosive classification (H314; CLP Annex I 3.3.2.1). ^{[3][8]}
Sensitisation	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) ^{[3][8]}
Mutagenicity	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) ^{[3][8]}
Carcinogenicity	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) ^{[3][8]}
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	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) ^{[3][8]}
STOT — single exposure	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) ^{[3][8]}
STOT — repeated exposure	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) ^{[3][8]}

12. Ecological information

Aquatic toxicity	Harmonised classification (CLP Annex VI): 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 = 2.6 ^[7] . Low bioaccumulation potential (log Kow < 4.5 — PBT/vPvB screening criterion per ECHA Guidance R.11). ^{[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



Class 6.1 — Toxic substances



Class 8 — Corrosive substances

UN number	UN 2261 ^[7]
Transport hazard class	Suggested from GHS classification — VERIFICATION REQUIRED.
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	UN number per the indicated source. Verify the transport class and packing group in ADR Table A / UN Model Regulations before shipment. ^[7]
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: harmonised under CLP Annex VI — Reg. (EC) No 1272/2008 (as at the date of issue). 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)

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Erkan SALAN. {-mAGIn} ZARF-FİİL EKİ ÜZERİNE. Journal of Turkish Research Institute (2015). DOI: 10.14222/turkiyat1364

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Full text of H statements

H311	Toxic in contact with skin
H301	Toxic if swallowed
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Full text of P statements

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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 ECHA harmonised classification (Annex VI to CLP, ATP 23).

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.
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- [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.
- [6] ISO. ISO 3864-1:2011 — Safety colours and safety signs. URL: <https://www.iso.org/standard/51021.html> Accessed: 2026-09-03.
- [7] PubChem. National Center for Biotechnology Information (NIH/NLM), chemical compound database. URL: <https://pubchem.ncbi.nlm.nih.gov/compound/10687>
- [8] ECHA. European Chemicals Agency — harmonised classification inventory (CLP Annex VI). URL: <https://echa.europa.eu>
- [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] 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>
- [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: 2026-09-03.

External links

NIST: <https://webbook.nist.gov/cgi/cbook.cgi?ID=1300-71-6>
ChEMBL: https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL1490403



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