SAFETY DATA SHEET (SDS)

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

Date: 21.10.2026 | Version: 5 | EN

2-(Cyclohexylthio)-1H-isoindole-1,3(2H)-dione

2-cyclohexylsulfanylisoindole-1,3-dione

CAS 17796-82-6

$C_{14}H_{15}NO_2S$ | EC 241-774-1

MOLAR MASS	LOGP
261.34	2.7

HAZARD CLASSIFICATION (GHS / CLP)



Danger

H317 | H410 | H318 | H351 | H400 | H319 | H373

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	2-(Cyclohexylthio)-1H-isoindole-1,3(2H)-dione
1.1 IUPAC name	2-cyclohexylsulfanylisoindole-1,3-dione
1.1 CAS number	17796-82-6
1.1 EC number	241-774-1
1.1 PubChem CID	28777
1.1 InChIKey	UEZWYKZHXASYJN-UHFFFAOYSA-N
1.1 SMILES	C1CCC(CC1)SN2C(=O)C3=CC=CC=C3C2=O
1.1 Molecular formula	$C_{14}H_{15}NO_2S$ [7]
1.1 Molar mass	261.34 g/mol [7]
1.1 Exact mass	261.0823 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:



Danger

Hazard statements (H) [3][4]

H317	May cause an allergic skin reaction
H410	Very toxic to aquatic life with long lasting effects
H318	Causes serious eye damage
H351	Suspected of causing cancer
H400	Very toxic to aquatic life
H319	Causes serious eye irritation
H373	May cause damage to organs through prolonged or repeated exposure

Precautionary statements (P) [3][4]

P201	Obtain special instructions before use
P202	Do not handle until all safety precautions have been read and understood
P260	Do not breathe dust/fume/gas/mist/vapours/spray
P264	Wash thoroughly after handling
P272	Contaminated work clothing should not be allowed out of the workplace
P273	Avoid release to the environment
P280	Wear protective gloves/protective clothing/eye protection/face protection
P302+P352	IF ON SKIN: Wash with plenty of water
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes; Remove contact lenses, if present and easy to do. Continue rinsing
P308+P313	IF exposed or concerned: Get medical advice/attention
P310	Immediately call a POISON CENTER or doctor/physician
P314	Get medical advice/attention if you feel unwell
P321	Specific treatment
P333+P313	If skin irritation or rash occurs: Get medical advice/attention
P337+P313	If eye irritation persists: Get medical advice/attention
P362+P364	Take off contaminated clothing
P391	Collect spillage
P405	Store locked up
P501	Dispose of contents/container to an approved waste collection point

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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	17796-82-6
EC number	241-774-1
Molecular formula	$C_{14}H_{15}NO_2S$
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. Call an ophthalmologist immediately. [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. Emergency number: 112 (EU-wide). Contact the poison centre designated in your country (CLP Art. 45). [1][2][10]

Symptoms and effects

eye irritation and watering. [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, NOx, SOx. [11]
Advice for firefighters	Use self-contained breathing apparatus (SCBA). Full protective suit.
Flash Point	177°C [7]

6. Accidental release measures

Personal precautions	Use personal protective equipment (see Section 8). Avoid breathing dust. [1][2][10]
Environmental precautions	Prevent entry into sewers, groundwater and surface water. [1][2][10]
Methods for containment and cleaning up	Collect mechanically into suitable containers. Absorption: sand, vermiculite, diatomaceous earth. Do not sweep dry (dust formation). [1][2][10]
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][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][14]



9. Physical and chemical properties

Property (item 9.1)	Value	Source
Physical state	Solid	
Colour	Off-white solid [7]	
Odour	No data available.	
pH (1% aqueous solution)	No data available.	
Melting point	92.6°C (experimental data) [7]	
Boiling point	196°C (experimental data) [7]	
Flash point	177°C (experimental data) [7]	
Flammability	No data available.	
Lower and upper explosion limit	Not applicable (REACH 9.1(g))	
Density (20°C)	1.33 g/cm³ [7]	
Vapour pressure	0 kPa (0 mmHg) (experimental data) [7]	
Relative vapour density	Not applicable (REACH 9.1(q))	
Kinematic viscosity	Not applicable (REACH 9.1(l))	

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Property (item 9.1)	Value	Source
Auto-ignition temperature	No data available.	
Decomposition temperature	Not applicable	
Water solubility	0.0108 g/L, 20°C [7]	
Particle characteristics	The particle size distribution has not been determined for this commercial form — required under Annex II 9.1(r); to be completed from the supplier's specification.	
Partition coefficient n-octanol/water (log value)	2.7 [8]	
Molar mass	261.34 g/mol [7]	
Molecular formula	$C_{14}H_{15}NO_2S$ [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, NOx, SOx.

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	Category 1 — serious eye damage.
Sensitisation	Skin, Category 1 (H317): May cause an allergic skin reaction. [3]
Mutagenicity	No data available.
Carcinogenicity	Classification from aggregated ECHA C&L notifications (non-harmonised) — requires verification; no entry in Annex VI to CLP.
IARC classification (carcinogenicity)	No individual IARC monograph — NOTE: substance classified as carcinogenic per ECHA CLP; absence of an IARC entry does NOT mean absence of carcinogenicity.
Reproductive toxicity	No data available.
STOT — single exposure	No data available.
STOT — repeated exposure	Category 2 (H373): May cause damage to organs through prolonged or repeated exposure. [3]
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)): H400 — Very toxic to aquatic life (Aquatic Acute 1); H410 — Very toxic to aquatic life with long lasting effects (Aquatic Chronic 1). 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 = 2.7 [8]. Low bioaccumulation potential (log Kow < 4.5 — PBT/vPvB screening criterion per ECHA Guidance R.11). [15][16]
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. [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	CLP classification (H400/H410) 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 21.10.2026 were omitted as future (not yet applicable).

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

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Scientific citations (8)

Geier J, Lessmann H, Frosch PJ et al.. *Contact sensitization to N-(cyclohexylthio)phthalimide.*. Contact dermatitis (2003).

Kanerva L, Estlander T, Jolanki R. *Allergic patch test reactions caused by the rubber chemical cyclohexyl thiophthalimide.*. Contact dermatitis (1996). DOI: 10.1111/j.1600-0536.1996.tb02106.x

Huygens S, Barbaud A, Goossens A. *Frequency and relevance of positive patch tests to cyclohexylthiophthalimide, a new rubber allergen.*. European journal of dermatology : EJD (2001).

Loffeld A, Foulds IS. *Allergic contact dermatitis from N-(cyclohexylthio) phthalimide in a playground fitter.*. Contact dermatitis (2004). DOI: 10.1111/j.0105-1873.2004.0424c.x

Slamenová D, Gábelová A, Chalupa I et al.. *Cytotoxic and genotoxic effect of inhibitor of vulcanisation N-cyclohexylthiophthalimide in a battery of in vitro assays.*. Mutation research (1999). DOI: 10.1016/s1383-5718(99)00146-1

Full text of H statements

H317	May cause an allergic skin reaction
H410	Very toxic to aquatic life with long lasting effects
H318	Causes serious eye damage
H351	Suspected of causing cancer
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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

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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

v5 (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.

[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/28777

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

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

[13] 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

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

[15] 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

[16] 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

[17] 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=17796-82-6

ChEMBL: https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL1532794

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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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