

According to the UN GHS revision 8

Creation Date: May 05, 2026

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1. IDENTIFICATION

1.1 GHS Product identifier

Product name: 3-Isopropenyl-alpha,alpha-dimethylbenzyl

Catalog Number: T7859

CAS Number: 2094-99-7

1.2 Other means of identification

Other names: -

1.3 Recommended use of the chemical and restrictions on use

Identified uses: no data available

1.4 Supplier's details

Company: Targetmol Chemicals Inc.

Address: 34 Washington Street, Wellesley Hills, Massachusetts 02481 USA

Tel/Fax: (781) 999-4286

1.5 Emergency phone number

Emergency phone number: 781-999-4286

Service hours: Monday to Friday, 9am-5pm (Standard timezone: UTC/GMT -5 hours).

2. HAZARD IDENTIFICATION

2.1 Classification of the substance or mixture

Skin corrosion, Sub-category 1B

Skin sensitization, Category 1

Serious eye damage, Category 1

Acute toxicity - Category 2, Inhalation

Respiratory sensitization, Category 1

Specific target organ toxicity - repeated exposure, Category 2

Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1

Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 1

2.2 GHS label elements, including precautionary statements

Pictogram(s):



Signal word:

Danger

Hazard statement(s):

H314 Causes severe skin burns and eye damage

H317 May cause an allergic skin reaction

H330 Fatal if inhaled

H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled

H373 May cause damage to organs through prolonged or repeated exposure

H410 Very toxic to aquatic life with long lasting effects

Precautionary statement(s):

Prevention:

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P264 Wash ... thoroughly after handling.

Response: P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
 P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
 P272 Contaminated work clothing should not be allowed out of the workplace.
 P271 Use only outdoors or in a well-ventilated area.
 P284 [In case of inadequate ventilation] wear respiratory protection.
 P273 Avoid release to the environment.

P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
 P363 Wash contaminated clothing before reuse.
 P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
 P316 Get emergency medical help immediately.
 P321 Specific treatment (see ... on this label).
 P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
 P302+P352 IF ON SKIN: Wash with plenty of water/...
 P333+P317 If skin irritation or rash occurs: Get medical help.
 P362+P364 Take off contaminated clothing and wash it before reuse.
 P305+P354+P338 IF IN EYES: Immediately rinse with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
 P317 Get medical help.
 P320 Specific treatment is urgent (see ... on this label).
 P342+P316 If experiencing respiratory symptoms: Get emergency medical help immediately.
 P319 Get medical help if you feel unwell.
 P391 Collect spillage.

Storage: P405 Store locked up.
 P403+P233 Store in a well-ventilated place. Keep container tightly closed.

Disposal: P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

2.3 Other hazards which do not result in classification

no data available

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number
3-Isopropenyl-alpha,alpha-dimethylbenzyl	-	2094-99-7	606-676-9

4. FIRST-AID MEASURES

4.1 Description of necessary first-aid measures

General advice

no data available

If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

4.2 Most important symptoms/effects, acute and delayed

no data available

4.3 Indication of immediate medical attention and special treatment needed, if necessary

no data available

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media

Use dry chemical, carbon dioxide or alcohol-resistant foam.

5.2 Specific hazards arising from the chemical

no data available

5.3 Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

6.2 Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

7.2 Conditions for safe storage, including any incompatibilities

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

Pure form: -20°C for 3 years | In solvent: -80°C for 1 year

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

8.2 Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

8.3 Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

9. PHYSICAL AND CHEMICAL PROPERTIES

Physical state	Solid
Color	no data available
Odour	no data available
Melting point/freezing point	180°C(dec.)(lit.)
Boiling point or initial boiling point and boiling range	268.4 °C. Atm. press.:101.3 kPa.
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	> 100 °C.
Auto-ignition temperature	448 °C.
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	DMSO: 2.02 mg/mL (10.04 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
N-octanol-water partition coefficient	log Pow = 5.4.
Vapour pressure	1.34 Pa. Temperature:25 °C.
Density and/or relative density	1.02.
Relative vapour density	no data available
Particle characteristics	no data available

10. STABILITY AND REACTIVITY

10.1 Reactivity

no data available

10.2 Chemical stability

no data available

10.3 Possibility of hazardous reactions

no data available

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

no data available

10.6 Hazardous decomposition products

no data available

11. TOXICOLOGICAL INFORMATION

Acute toxicity

Oral: LD50 - 3 400 mg/kg bw.

Inhalation: LC50 - 0.7 mg/L air.

Dermal: LD50 - > 2 000 mg/kg bw.

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

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

12.1 Toxicity

Toxicity to fish: LC50 - Pimephales promelas - 0.83 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - other aquatic crustacea: - 1.9 mg/L - 48 h.

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

12.2 Persistence and degradability

no data available

12.3 Bioaccumulative potential

no data available

12.4 Mobility in soil

no data available

12.5 Other adverse effects

no data available

13. DISPOSAL CONSIDERATIONS

13.1 Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

14. TRANSPORT INFORMATION

14.1 UN Number

no data available

14.2 UN Proper Shipping Name

no data available

14.3 Transport hazard class(es)

no data available

14.4 Packing group, if applicable

no data available

14.5 Environmental hazards

no data available

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to IMO instruments

no data available

15. REGULATORY INFORMATION

15.1 Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)	Not Listed.
EC Inventory	Not Listed.
United States Toxic Substances Control Act (TSCA) Inventory	Listed.
China Catalog of Hazardous chemicals 2015	Not Listed.
New Zealand Inventory of Chemicals (NZIoC)	Listed.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)	Not Listed.
Vietnam National Chemical Inventory	Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)	Listed.
Korea Existing Chemicals List (KECL)	Listed.

16. OTHER INFORMATION

Information on revision

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Abbreviations and acronyms

- CAS: Chemical Abstracts Service
- ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road
- RID: Regulation concerning the International Carriage of Dangerous Goods by Rail
- IMDG: International Maritime Dangerous Goods
- IATA: International Air Transportation Association
- TWA: Time Weighted Average
- STEL: Short term exposure limit
- LC50: Lethal Concentration 50%
- LD50: Lethal Dose 50%
- EC50: Effective Concentration 50%

References

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

Other Information

no data available

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