



# ISOPHORONE (3-METHYL-D3;2,4,4,6,6-D5,97%)

## Safety Data Sheet

according to Regulation (EC) No. 453/2010 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Date of issue: 30/03/2011

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Supersedes: 27/02/2012

Version: 3.0

**DLM-1943**

### SECTION 1: Identification of the substance/mixture and of the company/undertaking

#### 1.1. Product identifier

Product form : Substance  
Substance name : ISOPHORONE (3-METHYL-D3;2,4,4,6,6-D5,97%)  
EC index no : 606-012-00-8 (Unlabeled)  
EC no : 201-126-0 (Unlabeled)  
CAS No : 78-59-1 (Unlabeled)  
Product code : DLM-1943  
Formula : C9H6D8O

#### 1.2. Relevant identified uses of the substance or mixture and uses advised against

##### 1.2.1. Relevant identified uses

Industrial/Professional use spec : For professional use only.

##### 1.2.2. Uses advised against

No additional information available

#### 1.3. Details of the supplier of the safety data sheet

Cambridge Isotope Laboratories, Inc.  
50 Frontage Road  
Andover, MA 01810  
USA

USA: 1-800-322-1174 Int: 1-978-749-8000  
[cilsales@isotope.com](mailto:cilsales@isotope.com) [www.isotope.com](http://www.isotope.com)

#### Emergency telephone number

Emergency numbers:

Chemtrec: 1-800-424-9300 (24 hours)  
International: 1-703-741-5970 (24 hours)

### SECTION 2: Hazards identification

#### 2.1. Classification of the substance or mixture

##### Classification according to Regulation (EC) No. 1272/2008 [CLP]

Acute Tox. 4 (Oral) H302  
Acute Tox. 4 (Dermal) H312  
Eye Irrit. 2 H319  
Carc. 2 H351  
STOT SE 3 H335

Full text of H-phrases: see section 16

##### Classification according to Directive 67/548/EEC or 1999/45/EC

Carc.Cat.3; R40  
Xn; R21/22  
Xi; R36/37

Full text of R-phrases: see section 16

##### Classification (GHS-US)

Acute Tox. 4 (Oral) H302  
Acute Tox. 4 (Dermal) H312  
Eye Irrit. 2A H319  
Carc. 2 H351  
STOT SE 3 H335

#### Adverse physicochemical, human health and environmental effects

Lungs, Liver, Kidney, Central nervous system.

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### 2.2. Label elements

#### Labeling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP) :



GHS08

GHS07

Signal word (CLP) :

Warning

Hazard statements (CLP) :

H302+H312 - Harmful if swallowed or in contact with skin  
H319 - Causes serious eye irritation  
H335 - May cause respiratory irritation  
H351 - Suspected of causing cancer

Precautionary statements (CLP) :

P261 - Avoid breathing dust, fume, gas, mist, spray, vapors  
P264 - Wash both hands thoroughly after handling  
P270 - Do no eat, drink or smoke when using this product  
P271 - Use only outdoors or in a well-ventilated area  
P280 - Wear eye protection, face protection, protective clothing, protective gloves  
P301+P312 - IF SWALLOWED: Call a POISON CENTER/doctor/.../if you feel unwell  
P302+P352 - IF ON SKIN: Wash with plenty of water/...  
P304+P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing

#### GHS-US labeling

Hazard pictograms (GHS-US) :



GHS08

GHS07

Signal word (GHS-US) :

Warning

Hazard statements (GHS-US) :

H302+H312 - Harmful if swallowed or in contact with skin  
H319 - Causes serious eye irritation  
H335 - May cause respiratory irritation  
H351 - Suspected of causing cancer (Dermal, Inhalation, oral)

Precautionary statements (GHS-US) :

P201 - Obtain special instructions before use  
P202 - Do not handle until all safety precautions have been read and understood  
P261 - Avoid breathing dust, fume, gas, mist, spray, vapors  
P264 - Wash Both hands thoroughly after handling  
P270 - Do no eat, drink or smoke when using this product  
P271 - Use only outdoors or in a well-ventilated area  
P280 - Wear eye protection, face protection, protective clothing, protective gloves  
P301+P312 - IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell  
P302+P352 - IF ON SKIN: Wash with plenty of soap and water  
P304+P340 - IF INHALED: Remove victim to fresh air and keep at rest in a position 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  
P308+P313 - IF exposed or concerned: Get medical advice/attention  
P312 - Call a POISON CENTER/doctor/physician if you feel unwell  
P321 - Specific treatment (see Hazard pictograms (CLP) on this label)  
P330 - If swallowed, rinse mouth  
P337+P313 - If eye irritation persists: Get medical advice/attention  
P362+P364 - Take off contaminated clothing and wash it before reuse  
P403+P233 - Store in a well-ventilated place. Keep container tightly closed  
P405 - Store locked up  
P501 - Dispose of contents/container to Comply with applicable regulations.

### 2.3. Other hazards

No additional information available

## SECTION 3: Composition/information on ingredients

### 3.1. Substances

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Name	Product identifier	%	Classification according to Directive 67/548/EEC
ISOPHORONE (3-METHYL-D3;2,4,4,6,6-D5,97%) (Main constituent)	(CAS No) 78-59-1 (Unlabeled) (EC no) 201-126-0 (Unlabeled) (EC index no) 606-012-00-8 (Unlabeled)	100	Carc.Cat.3; R40 Xn; R21/22 Xi; R36/37

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
ISOPHORONE (3-METHYL-D3;2,4,4,6,6-D5,97%) (Main constituent)	(CAS No) 78-59-1 (Unlabeled) (EC no) 201-126-0 (Unlabeled) (EC index no) 606-012-00-8 (Unlabeled)	100	Acute Tox. 4 (Oral), H302 Acute Tox. 4 (Dermal), H312 Eye Irrit. 2, H319 Carc. 2, H351 STOT SE 3, H335

Full text of R-, H- and EUH-phrases: see section 16

Name	Product identifier	%	Classification (GHS-US)
ISOPHORONE (3-METHYL-D3;2,4,4,6,6-D5,97%) (Main constituent)	(CAS No) 78-59-1 (Unlabeled)	100	Acute Tox. 4 (Oral), H302 Acute Tox. 4 (Dermal), H312 Eye Irrit. 2A, H319 Carc. 2, H351 STOT SE 3, H335

Full text of H-phrases: see section 16

### 3.2. Mixtures

Not applicable

## SECTION 4: First aid measures

### 4.1. Description of first aid measures

- First-aid measures general : Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.
- First-aid measures after inhalation : If breathed in, move person to fresh air. If not breathing, give artificial respiration. Consult a physician.
- First-aid measures after skin contact : Wash with soap and plenty of water. Consult a physician.
- First-aid measures after eye contact : Flush eye with water for 15 minutes. Get medical attention.
- First-aid measures after ingestion : Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

### 4.2. Most important symptoms and effects, both acute and delayed

- Symptoms/injuries after inhalation : May be harmful if inhaled. Causes respiratory tract irritation.
- Symptoms/injuries after skin contact : Harmful if absorbed through skin. Causes skin irritation.
- Symptoms/injuries after eye contact : Causes eye irritation.
- Symptoms/injuries after ingestion : Harmful if swallowed.

### 4.3. Indication of any immediate medical attention and special treatment needed

No additional information available

## SECTION 5: Firefighting measures

### 5.1. Extinguishing media

- suitable extinguishing media : Use water spray, alcohol-resistant foam, dry chemical, or carbon dioxide.

### 5.2. Special hazards arising from the substance or mixture

No additional information available

### 5.3. Advice for firefighters

- Protection during firefighting : Do not enter fire area without proper protective equipment, including respiratory protection.

## SECTION 6: Accidental release measures

### 6.1. Personal precautions, protective equipment and emergency procedures

#### 6.1.1. For non-emergency personnel

- Emergency procedures : Use personal protective equipment. Avoid breathing vapors, mist, or gas. Ensure adequate ventilation.

#### 6.1.2. For emergency responders

No additional information available

### 6.2. Environmental precautions

Do not let product enter drains.

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### 6.3. Methods and material for containment and cleaning up

For containment : Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

### 6.4. Reference to other sections

No additional information available

## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

Additional hazards when processed : Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Normal measures for preventive fire protection.

Hygiene measures : Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

### 7.2. Conditions for safe storage, including any incompatibilities

Storage conditions : Store at room temperature away from light and moisture.

### 7.3. Specific end use(s)

No additional information available

## SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

ISOPHORONE (3-METHYL-D3;2,4,4,6,6-D5,97%) (78-59-1 (Unlabeled))		
Italy - Portugal - USA ACGIH	ACGIH TWA (ppm)	5 ppm Central Nervous System impairment; Upper Respiratory Tract irritation; Eye irritation; Malaise; Fatigue; Confirmed animal carcinogen with unknown relevance to humans
USA NIOSH	NIOSH REL (TWA) (mg/m3)	23 The value in mg/m3 is approximate.
USA NIOSH	NIOSH REL (TWA) (ppm)	4 ppm
USA OSHA	OSHA PEL (TWA) (mg/m3)	140 The value in mg/m3 is approximate.
USA OSHA	OSHA PEL (TWA) (ppm)	25 ppm

### 8.2. Exposure controls

Personal protective equipment : Safety glasses. Gloves. Respiratory protection of the dependent type. Protective clothing.



Hand protection : Wear suitable protective clothing and gloves.

Eye protection : Wear safety glasses with side shields (or goggles) and a face shield.

Skin and body protection : Choose body protection according to the amount and concentration of the dangerous substance at the work place.

Respiratory protection : When appropriate, use NIOSH/CEN approved respirator.

## SECTION 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

Physical state	: Liquid
Appearance	: Liquid, clear.
Molecular mass	: 146.26 g/mol (Unlabeled)
Color	: Light yellow.
Odor	: No data available
Odor threshold	: No data available
pH	: No data available
Relative evaporation rate (butyl acetate=1)	: No data available
Melting point	: -8 °C (18 °F) - lit
Freezing point	: No data available
Boiling point	: 213 - 214 °C (415 - 417 °F) - lit
Flash point	: 96.0 °C (204.8 °F) - closed cup
Self ignition temperature	: 462 °C (863.6 °F)
Decomposition temperature	: No data available
Flammability (solid, gas)	: No data available
Vapor pressure	: 1.3 hPa (1.0 mmHg) at 38.0 °C (100.4 °F)

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Relative vapor density at 20 °C	: No data available
Relative density	: No data available
Density	: 0.923 g/ml at 25.0 °C (77 °F)
Solubility	: No data available
Log Pow	: No data available
Log Kow	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available
Explosive limits	: 0.8 - 3.8 % (V)

### 9.2. Other information

No additional information available

## SECTION 10: Stability and reactivity

### 10.1. Reactivity

No additional information available

### 10.2. Chemical stability

Stable if stored under recommended conditions.

### 10.3. Possibility of hazardous reactions

No additional information available

### 10.4. Conditions to avoid

Not available.

### 10.5. Incompatible materials

Strong oxidizing agents, Strong acids, Strong bases.

### 10.6. Hazardous decomposition products

formed under fire conditions: Carbon oxides.

## SECTION 11: Toxicological information

### 11.1. Information on toxicological effects

Acute toxicity : Harmful if swallowed. Harmful in contact with skin.

ISOPHORONE (3-METHYL-D3;2,4,4,6,6-D5,97%) (78-59-1 (Unlabeled))	
LD50 oral rat	1870 mg/kg
LD50 dermal rabbit	1382 mg/kg
ATE (oral)	1870.000 mg/kg body weight
ATE (dermal)	1382.000 mg/kg body weight

Skin corrosion/irritation	: Not classified Skin - rabbit - Mild skin irritation - 24 h
Serious eye damage/irritation	: Causes serious eye irritation. Eyes - rabbit - Eye irritation - 24 h
Respiratory or skin sensitization	: Not available No data available
Germ cell mutagenicity	: Not available
Carcinogenicity	: This product is or contains a component that has been reported to be possibly carcinogenic based on its IARC, ACGIH, NTP, or EPA classification. Limited evidence of carcinogenicity in animal studies.
Reproductive toxicity	: Not available
Specific target organ toxicity (single exposure)	: May cause respiratory irritation. No data available
Specific target organ toxicity (repeated exposure)	: Not classified No data available
Aspiration hazard	: Not classified
Potential Adverse human health effects and symptoms	: Burning sensation. Cough. Wheezing. Shortness of breath. Headache. Nausea. Vomiting. Central nervous system depression. Narcosis.
Symptoms/injuries after inhalation	: May be harmful if inhaled. Causes respiratory tract irritation.
Symptoms/injuries after skin contact	: Harmful if absorbed through skin. Causes skin irritation.

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Symptoms/injuries after eye contact : Causes eye irritation.  
Symptoms/injuries after ingestion : Harmful if swallowed.

### SECTION 12: Ecological information

#### 12.1. Toxicity

ISOPHORONE (3-METHYL-D3;2,4,4,6,6-D5,97%) (78-59-1 (Unlabeled))	
LC50 fish 1	145 mg/l Pimephales promelas (fathead minnow) - 96 h
EC50 Daphnia 1	120 mg/l Daphnia magna (Water flea) - 48 h
NOEC (chronic)	170 mg/l Cyprinodon variegatus (sheephead minnow) - 96 h

#### 12.2. Persistence and degradability

ISOPHORONE (3-METHYL-D3;2,4,4,6,6-D5,97%) (78-59-1 (Unlabeled))	
Persistence and degradability	Not available.

#### 12.3. Bioaccumulative potential

ISOPHORONE (3-METHYL-D3;2,4,4,6,6-D5,97%) (78-59-1 (Unlabeled))	
BCF fish 1	0.0924 mg/l Lepomis macrochirus (Bluegill) - 14d
Bioconcentration factor (BCF REACH)	7

#### 12.4. Mobility in soil

ISOPHORONE (3-METHYL-D3;2,4,4,6,6-D5,97%) (78-59-1 (Unlabeled))	
Ecology - soil	Not available.

#### 12.5. Results of PBT and vPvB assessment

No additional information available

#### 12.6. Other adverse effects

Other adverse effects : Not available.

### SECTION 13: Disposal considerations

#### 13.1. Waste treatment methods

Regional legislation (waste) : Waste materials should be disposed of under conditions which meet Federal, State, and Local environmental control regulations.  
Waste disposal recommendations : Dispose in a safe manner in accordance with local/national regulations.

### SECTION 14: Transport information

In accordance with ADR / RID / ADNR / IMDG / ICAO / IATA

#### 14.1. UN number

UN-No.(DOT) : 3082  
DOT NA no. UN3082

#### 14.2. UN proper shipping name

DOT Proper Shipping Name : Environmentally hazardous substances, liquid, n.o.s.  
Department of Transportation (DOT) Hazard Classes : 9 - Class 9 - Miscellaneous hazardous material 49 CFR 173.140  
Hazard labels (DOT) : 9 - Class 9 (Miscellaneous dangerous materials)



DOT Symbols : G - Identifies PSN requiring a technical name  
Packing group (DOT) : III - Minor Danger

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DOT Special Provisions (49 CFR 172.102)	: 8 - A hazardous substance that is not a hazardous waste may be shipped under the shipping description "Other regulated substances, liquid or solid, n.o.s.", as appropriate. In addition, for solid materials, special provision B54 applies. 146 - This description may be used for a material that poses a hazard to the environment but does not meet the definition for a hazardous waste or a hazardous substance, as defined in 171.8 of this subchapter, or any hazard class as defined in Part 173 of this subchapter, if it is designated as environmentally hazardous by the Competent Authority of the country of origin, transit or destination. 173 - An appropriate generic entry may be used for this material. 335 - Mixtures of solids that are not subject to this subchapter and environmentally hazardous liquids or solids may be classified as "Environmentally hazardous substances, solid, n.o.s.," UN3077 and may be transported under this entry, provided there is no free liquid visible at the time the material is loaded or at the time the packaging or transport unit is closed. Each transport unit must be leak-proof when used as bulk packaging. IB3 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1 and 31HA2, 31HB2, 31HN2, 31HD2 and 31HH2). Additional Requirement: Only liquids with a vapor pressure less than or equal to 110 kPa at 50 C (1.1 bar at 122 F), or 130 kPa at 55 C (1.3 bar at 131 F) are authorized, except for UN2672 (also see Special Provision IP8 in Table 2 for UN2672). T4 - 2.65 178.274(d)(2) Normal..... 178.275(d)(3) TP1 - The maximum degree of filling must not exceed the degree of filling determined by the following: Degree of filling = $97 / 1 + a (tr - tf)$ Where: tr is the maximum mean bulk temperature during transport, and tf is the temperature in degrees celsius of the liquid during filling. TP29 - A portable tank having a minimum test pressure of 1.5 bar (150.0 kPa) may be used provided the calculated test pressure is 1.5 bar or less based on the MAWP of the hazardous materials, as defined in 178.275 of this subchapter, where the test pressure is 1.5 times the MAWP.
DOT Packaging Exceptions (49 CFR 173.xxx)	: 155
DOT Packaging Non Bulk (49 CFR 173.xxx)	: 203
DOT Packaging Bulk (49 CFR 173.xxx)	: 241
DOT RQ	: 5000 lbs
Marine pollutant	: No

### 14.3. Additional information

Other information	: No supplementary information available.
Special transport precautions	: IMDG/IATA - Not dangerous goods.

#### Overland transport

Packing group (ADR)	: III
Class (ADR)	: 9 - Miscellaneous dangerous substances and articles
Hazard identification number (Kemler No.)	: 90
Classification code (ADR)	: M6
Danger labels (ADR)	: 9 - Miscellaneous dangerous compounds



Orange plates	: 
Tunnel restriction code	: E
Limited quantities (ADR)	: 5L
EAC	: •3Z
Excepted quantities (ADR)	: E1

#### Transport by sea

DOT Vessel Stowage Location	: A - The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel.
MFAG-No	: 171

#### Air transport

DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27)	: No limit
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DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75) : No limit  
Civil Aeronautics Law : Miscellaneous dangerous substances & articles

### 14.4. Environmental hazards

Other information : No supplementary information available.

### 14.5. Special precautions for user

Special transport precautions : IMDG/IATA - Not dangerous goods.

### 14.6. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable

## SECTION 15: Regulatory information

### 15.1. US Federal regulations

#### ISOPHORONE (3-METHYL-D3;2,4,4,6,6-D5,97%) (78-59-1 (Unlabeled))

SARA Section 311/312 Hazard Classes	Immediate (acute) health hazard
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### 15.2. International regulations

#### CANADA

#### ISOPHORONE (3-METHYL-D3;2,4,4,6,6-D5,97%) (78-59-1 (Unlabeled))

Listed on the Canadian DSL (Domestic Substances List) inventory.

#### 15.2.1. National regulations

No additional information available

### 15.3. US State regulations

#### ISOPHORONE (3-METHYL-D3;2,4,4,6,6-D5,97%)(78-59-1 (Unlabeled))

State or local regulations	U.S. - Massachusetts - Right To Know List U.S. - Pennsylvania - RTK (Right to Know) List U.S. - New Jersey - Right to Know Hazardous Substance List This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.
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## SECTION 16: Other information

Other information : This product is not radioactive. The data given for this product are those of the corresponding unlabeled compound, unless specifically indicated otherwise. Health and safety data for labeled compounds are generally not available, but are assumed to be similar or identical to the corresponding unlabeled compound.

Full text of R-, H- and EUH-phrases::

Acute Tox. 4 (Dermal)	Acute toxicity (dermal) Category 4
Acute Tox. 4 (Oral)	Acute toxicity (oral) Category 4
Carc. 2	Carcinogenicity Category 2
Eye Irrit. 2	Serious eye damage/eye irritation Category 2
STOT SE 3	Specific target organ toxicity (single exposure) Category 3
H302	Harmful if swallowed
H312	Harmful in contact with skin
H319	Causes serious eye irritation
H335	May cause respiratory irritation
H351	Suspected of causing cancer
R21/22	Harmful in contact with skin and if swallowed
R36/37	Irritating to eyes and respiratory system
R40	Limited evidence of a carcinogenic effect
Xi	Irritant
Xn	Harmful



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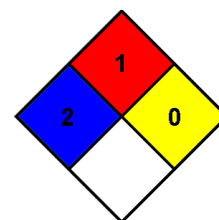
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NFPA health hazard : 2 - Intense or continued exposure could cause temporary incapacitation or possible residual injury unless prompt medical attention is given.

NFPA fire hazard : 1 - Must be preheated before ignition can occur.

NFPA reactivity : 0 - Normally stable, even under fire exposure conditions, and are not reactive with water.



### HMIS III Rating

Health : 2 Moderate Hazard - Temporary or minor injury may occur

Flammability : 1 Slight Hazard

Physical : 0 Minimal Hazard

### CIL Multi-Solvent Mixture SDS

*This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product*