

**Product:** **ISOPHORONE**

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SDS No.: 000166-001 (Version 2.2 )

Date 01.06.2015

**1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING**

**Substance name:**

REACH Registration Name: isophorone  
REACH Registration Number: 01-2119497282-32-0002  
EC Nr: 201-126-0  
CAS-No.: 78-59-1

**Use of the Substance/Mixture :**

Sector of use :	Product category :
Formulation and (re)packing of substances and mixtures <b>SU8:</b> Manufacture of bulk, large scale chemicals (including petroleum products), <b>SU 10:</b> Formulation [mixing] of preparations and/ or re-packaging (excluding alloys)	<b>All</b>
Use in coating (industrial)	<b>All</b>
Use in coating (professional)	<b>All</b>
Use in cleaning products (industrial)	<b>All</b>
Use in cleaning products (professional)	<b>All</b>
Use in agrochemicals <b>SU1:</b> Agriculture, forestry, fishery	<b>PC27:</b> Plant protection products
Industrial use as laboratory reagent	<b>All</b>
Professional use as laboratory reagent	<b>All</b>

**Company/Undertaking Identification:**

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**2. HAZARDS IDENTIFICATION**

**Classification (Regulation (EC) No 1272/2008):**

Oral: Acute toxicity, 4, H302  
Dermal: Acute toxicity, 4, H312  
Eye irritation, 2, H319  
Specific target organ toxicity - single exposure, 3, H335  
Carcinogenicity, 2, H351

**Classification (Directive 67/548/EEC):**

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

**Additional information:**

For the full text of the R, H, EUH-phrases mentioned in this Section, see Section 16.

**Label elements (REGULATION (EC) No 1272/2008):**

**Hazardous components which must be listed on the label:**

No. in ANNEXE : 606-012-00-8

3,5,5-trimethylcyclohex-2-enone; isophorone

Hazard pictograms:



Signal word:

**Warning**

Hazard statements:

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

Precautionary statements:

**Prevention:**

- P202 : Do not handle until all safety precautions have been read and understood.
- P261 : Avoid breathing gas/mist/vapours/spray.
- P281 : Use personal protective equipment as required.

**Response:**

- P308 + P313 : IF exposed or concerned: Get medical advice/ attention.

**Storage:**

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

**Other hazards:**

**Potential health effects:**

- Irritation: Irritating to nasal mucous membranes
- Inhalation: At high vapour/mist concentrations headache Drowsiness
- Skin contact: Slightly irritating to skin.
- Eye contact: Irritating to eyes.
- Chronic exposure: Limited evidence of a carcinogenic effect.

**Environmental Effects:**

- Readily biodegradable. Not bioaccumulable. In its normal state, this product does not present any specific risk for the environment.

**Physical and chemical hazards:**

- Flammable (when hot). Thermal decomposition giving toxic products
- Decomposition products: See chapter 10

**Other:**

- Results of PBT and vPvB assessment : According to REACH regulation, annex XIII, the substance does not meet PBT and vPvB criteria.

**3. COMPOSITION/INFORMATION ON INGREDIENTS**

Chemical name of the substance<sup>1</sup>: ISOPHORONE

Chemical Name <sup>1</sup>	EC-No.	CAS-No.	Concentration	Classification Directive 67/548/EEC	Classification Regulation (EC) No 1272/2008
Isophorone	201-126-0	78-59-1	>= 98,5 %	Carc.Cat.3; R40 Xn; R21/22 Xi; R36/37	Acute Tox. 4 (Oral); H302 Acute Tox. 4 (Dermal); H312 Eye Irrit. 2; H319 STOT SE 3; H335 Carc. 2; H351

<sup>1</sup>: See chapter 14 for Proper Shipping Name

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#### 4. FIRST AID MEASURES

##### Description of necessary first-aid measures, Most important symptoms/effects, acute and delayed:

**General advice:**

Take off immediately all contaminated clothing.

**Inhalation:**

Move to fresh air. Oxygen or artificial respiration if needed. Keep under medical surveillance. In case of problems : Hospitalise.

**Skin contact:**

Wash immediately, abundantly and thoroughly with water. If significant contact: Keep under medical surveillance. Hospitalise.

**Eye contact:**

Wash well-open eyes immediately, abundantly and thoroughly with water. Consult an ophthalmologist.

**Ingestion:**

In case of problems : Consult a doctor. If the subject is unconscious, do not induce vomiting Hospitalise.

**Protection of first-aiders:**

In case of insufficient ventilation, wear suitable respiratory equipment. Protective suit

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#### 5. FIREFIGHTING MEASURES

##### Extinguishing media:

**Suitable extinguishing media:** Water spray, Carbon dioxide (CO<sub>2</sub>), Foam, Dry powder

**Unsuitable extinguishing media:** High volume water jet

##### Special hazards arising from the substance or mixture:

Possible re-ignition of vapours from a distance, Thermal decomposition giving flammable and toxic products

##### Advice for firefighters:

**Specific methods:**

Cool containers / tanks with water spray. In case of fire nearby, remove exposed containers.

**Special protective actions for fire-fighters:**

Wear self-contained breathing apparatus and protective suit.

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#### 6. ACCIDENTAL RELEASE MEASURES

##### Personal precautions, protective equipment and emergency procedures:

Prohibit all sources of sparks and ignition - Do not smoke. Prohibit contact with skin and eyes and inhalation of vapours. Evacuate area of all unnecessary personnel. Wear personal protective equipment.

##### Environmental precautions:

Do not release into the environment. Do not let product enter drains. Dam up with sand or inert earth (do not use combustible materials).

##### Methods and materials for containment and cleaning up:

**Recovery:**

Pump into a labelled inert emergency tank. Absorb the remainder with an inert absorbent material. After cleaning, flush away traces with water. Recover waste water for processing later.

**Elimination:**

Destroy the product by incineration (in accordance with local and national regulations). Destroy absorbed product by incineration at an approved waste disposal site only In accordance with local and national regulations. Dispose of rinse water as waste water.

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#### 7. HANDLING AND STORAGE

##### Precautions for safe handling:

**Technical measures/Precautions:**

Storage and handling precautions applicable to products: Liquid. Flammable (when hot). Harmful. Irritant. With vapours explosive in air. Provide appropriate exhaust ventilation at machinery. Provide showers, eye-baths. Provide water supplies near the point of use. Provide self-contained breathing apparatus nearby.

**Safe handling advice:**

Keep well away from naked flames. Prohibit all sources of sparks and ignition - Do not smoke. Only use safety equipment.

**Hygiene measures:**

Avoid contact with the skin and the eyes. Avoid inhalation of vapours. When using do not eat, drink or smoke.  
Wash hands after handling. Remove contaminated clothing and protective equipment before entering eating areas.

**Conditions for safe storage, including any incompatibilities:**

Keep containers tightly closed in a cool, well-ventilated place. Keep away from heat and sources of ignition. Do not smoke. Provide a catch-tank in a bunded area. Provide electrical earthing of equipment and electrical equipment usable in explosive atmospheres.

Storage temperature: < 50 °C

**Incompatible products:**

Strong oxidizing agents, strong bases

**Packaging material:**

**Recommended:** Stainless steel, Ordinary steel

**To be avoided:** Plastic materials, Rubber, Aluminium, Galvanized steel

**Specific use(s) (End Use):** None.

**8. EXPOSURE CONTROLS/PERSONAL PROTECTION**

**CONTROL PARAMETERS:**

**Exposure Limit Values**

**Isophorone**

Source	Date	Value type	Value (ppm)	Value (mg/m3)	Remarks
ACGIH (US)	2007	Ceiling	5	-	-

**Derived No Effect Level (DNEL):**

End Use	Inhalation	Ingestion	Skin contact
Workers	22 mg/m3 (ST, SE, LE) 11 mg/m3 (LT, SE, LE)		41 mg/kg bw/day (ST, SE) 20,5 mg/kg bw/day (LT, SE)

**LE** : Local effects, **SE** : Systemic effects, **LT** : Long term, **ST** : Short term

**Predicted No Effect Concentration (PNEC):**

Compartment:	Value:
Water	0,089 mg/l
Marine water	0,0089 mg/l
Water (Intermittent release)	1,2 mg/l
Effects on waste water treatment plants	1 mg/l
Sediment	0,839 mg/kg dw
Marine sediment	0,0839 mg/kg dw
Soil	0,12 mg/kg dw
Oral (Secondary Poisoning)	0,02 mg/kg food

**EXPOSURE CONTROLS:**

**General protective measures:**

Ensure sufficient air exchange and/or exhaust in work areas

**Personal protective equipment:**

Respiratory protection:

Low concentrations or short activity: Self contained Breathing Apparatus  
High concentrations or prolonged activity: Self contained Breathing Apparatus  
PVC gloves

Hand protection:

According to permeation index EN 374: 1 (time elapsed > 10 mins)

Eye/face protection:

Safety glasses

Skin and body protection:

At the workplace : Protective clothing (cotton)

Intervention at incident: Protective clothing (cotton)

**Environmental exposure controls:** See chapter 6

**9. PHYSICAL AND CHEMICAL PROPERTIES**

**Appearance:**

**Physical state (20°C):**

liquid

**Colour:**

light yellow

**Odour:**

Smelling of camphor

<b>Olfactory threshold:</b>	0,2 ppm
<b>pH:</b>	No data available.
<b>Melting point/range :</b>	-8,1 °C
<b>Formation of an azeotrope with water</b> :	
<b>Boiling point/boiling range :</b>	215,3 °C (Pressure 1.013 hPa)
<b>Flash point:</b>	closed cup: 80 - 85 °C (Standard NF T 60 103)
<b>Evaporation rate:</b>	No data available.
<b><u>Flammability (solid, gas):</u></b>	
Lower flammable limit :	0,8 %(V)
Upper flammable limit :	3,8 %(V)
<b>Vapour pressure:</b>	0,4 hPa , at 20 °C
<b>Vapour density:</b>	5,7 kg/m <sup>3</sup>
<b>Density:</b>	920 kg/m <sup>3</sup> , at 20 °C
<b>Relative density (Water=1):</b>	0,92 at 20 °C
<b>Water solubility:</b>	12 g/l 40 g/l Solubility of water in the product
<b>Partition coefficient: n-octanol/water:</b>	log Kow : 1,67 , at 20 °C (OECD Test Guideline 107)
<b>Autoignition temperature:</b>	462 °C (Standard : BS 4056 1966)
<b>Decomposition temperature:</b>	No data available.
<b>Viscosity, dynamic:</b>	2,62 mPa.s , at 20 °C
<b><u>Explosive properties:</u></b>	
Explosivity:	Not relevant (due to the chemical structure)
<b>Oxidizing properties:</b>	Not relevant (due to the chemical structure)
<b><u>Other data:</u></b>	
<b>Solubility in other solvents:</b>	Soluble in most organic solvents
<b>Surface tension:</b>	32,3 mN/m Surface tension
<b>Henry constant:</b>	380E-03 Pa.m <sup>3</sup> /mol
<b>Molecular Weight:</b>	138,2 g/mol
<b>Refractive index:</b>	1,476 at 20 °C

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## 10. STABILITY AND REACTIVITY

### Reactivity & Chemical stability:

No data available.

### Conditions to avoid:

Keep away from heat and sources of ignition.

### Incompatible materials to avoid:

Strong oxidizing agents, Hydrogen peroxide, Nitric acid, Bases, (under certain conditions of temperature and pressure), Polymerisation can occur.

### Hazardous decomposition products:

Thermal decomposition giving toxic products, Carbon monoxide

### Further information:

The product is stable under normal handling and storage conditions.

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## 11. TOXICOLOGICAL INFORMATION

### Toxicokinetics (absorption, metabolism, distribution and elimination):

A big quantity of product can be quickly absorbed through all routes. It is distributed in the whole body.

### Toxicological information:

### Acute toxicity:

**Inhalation:** Slightly harmful by inhalation

- In man : At high vapour/mist concentrations, Risk of, headache, Drowsiness, narcosis, Suffocation
- In animals : LC50/4 h/rat: 7 mg/l (Aerosol)

- Ingestion:** **Harmful if swallowed.**
- In animals : LD50/rat: 1.500 - 3.450 mg/kg

- Dermal:** **Harmful in contact with skin.**
- In animals : LD50/rat: 1.700 mg/kg

**Local effects ( Corrosion / Irritation / Serious eye damage ):**

- Skin contact:** **Slightly irritating to skin.**
- In animals : Mild skin irritation (OECD Test Guideline 404, rabbit, Exposure time: 4 h)

- Eye contact:** **Irritating to eyes.**
- In man : Exposure to vapours, Eye irritation (0,37 mg/l)
  - In animals : Eye irritation (Draize Test, rabbit)

**Respiratory or skin sensitization:**

- Inhalation:** No data available.

- Skin contact:** **Not a skin sensitizer**
- In animals : No skin allergy was observed (Method : OECD Test Guideline 406 Guinea pig maximization test)

**CMR effects :**

- Mutagenicity:** **According to available experimental data: Overall not genotoxic**

**In vitro**

Ames test in vitro: Inactive  
Tests for chromosome aberrations in vitro on mammalian cells: Inactive  
In vitro gene mutations test on mammalian cells: Inconclusive results

**In vivo**

Micronucleus test in vivo mouse: Inactive

- Carcinogenicity:** **According to available experimental data: The tumour-inducing effects on the liver observed at high doses in rats and mice are specific to these animal species and are considered as unsuitable for extrapolation to man.**

- In animals : At high doses : Liver tumours (mouse) - Kidney tumours (rat) (2 years, By oral route)

**Reproductive toxicity:**

- Fertility:** **According to limited available data Absence of toxic effects on fertility**

- In animals : Reproduction Test: No toxic effects for reproduction  
NOAEL ( Parent ): < 2,87 mg/l  
NOAEL ( F1 ): 2,87 mg/l (rat, By inhalation)  
Absence of toxic effects upon the reproductive system, NOAEL: 1000 mg/kg (rat, mouse, By oral route, 3 mois)

- Foetal development:** **According to available experimental data: Absence of toxic effects for foetal development.**

- In animals : Exposure during pregnancy: Absence of toxic effects for foetal development., NOAEL: 0,66 mg/l  
Maternal concentration without effect: 0,29 mg/l (Method: OECD Test Guideline 414, rat, mouse, By inhalation)

**Specific target organ toxicity :**

**Single exposure :**

**Irritating to respiratory system.**  
Exposure routes : Inhalation  
Target Organs : Upper respiratory tract

**Inhalation:**

• In man :

Olfactory threshold: 0,2 ppm  
Exposure to vapours  
Irritation (throat) (0,20 mg/l)  
Irritating to nasal mucous membranes (0,37 mg/l)

**Repeated exposure:**

• In animals :

**The substance or mixture is not classified as specific target organ toxicant, repeated exposure.**  
By inhalation: Concentration has no effect on nasal mucous membranes  
> 0,51 mg/l (mouse, 2 Weeks)  
By oral route: No specific toxic effects  
NOAEL= > 233mg/kg bw/day (rat, 13 Weeks)

**Aspiration hazard:**

Not applicable

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**12. ECOLOGICAL INFORMATION**

**Acute toxicity**

**Fish:**

**Practically nontoxic.**  
LC50, 96 h (Pimephales promelas (fathead minnow)) : 228 mg/l (Test substance: Active ingredient)

**Aquatic invertebrates:**

**Practically nontoxic**  
EC(l)50, 48 h (Daphnia magna (Water flea)) : 120 mg/l (Method: US EPA, Immobilization, Test substance: Active ingredient)

**Aquatic plants:**

**Practically nontoxic.**  
IC50, 72 h (Desmodesmus subspicatus (green algae)) : 475,4 mg/l (Test substance: Active ingredient)  
NOEC : 64 mg/l

**Microorganisms:**

**Practically nontoxic**  
EC10, 18 h (Pseudomonas putida) : 328 mg/l (Method: no data available, Growth inhibition, Test substance: Active ingredient)  
EC50, 3 h (Activated sludge) : 100 mg/l (Method: OECD Test Guideline 209, Respiration inhibition, Test substance: Active ingredient)

**Aquatic toxicity / Long term toxicity:**

**Fish:**

No effect concentration, 35 d (Pimephales promelas (fathead minnow)) : 11 mg/l (Method: OECD Test Guideline 210, Test substance: Active ingredient)  
  
Lowest observed effect concentration : 19 mg/l

**Persistence and degradability :**

**Biodegradation (In water):**

**Readily biodegradable**  
95 % after 28 d (Method: OECD Test Guideline 301 A)

**Bioaccumulative potential :**

**Bioaccumulation:**

**Does not bioaccumulate.**  
Partition coefficient: n-octanol/water: log Kow : 1,67 , at 20 °C (Method: OECD Test Guideline 107)  
Bioconcentration factor (BCF): 1,1 - 1,8 (42 d, Method: OECD Test Guideline 305 C, Cyprinus carpio (Carp), Test substance: Active ingredient) Fish

**Mobility in soil - Distribution among environmental compartments:**

**Distribution among environmental compartments :**

Water: 87,6 %  
Air: 11,7 %  
(Method: Calculation according Mackay, Level I)

**Henry constant:**

380E-03 Pa.m<sup>3</sup>/mol

**Surface tension:**

32,3 mN/m Surface tension

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**Absorption / desorption:**

Non adsorbable , Koc: 77 ( Method: calculated )

**Results of PBT and vPvB assessment :**

According to REACH regulation, annex XIII, the substance does not meet PBT and vPvB criteria.

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**13. DISPOSAL CONSIDERATIONS**

**Waste treatment:**

**Disposal of product:** Destroy the product by incineration (in accordance with local and national regulations).

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**14. TRANSPORT INFORMATION**

Not classified as dangerous in the meaning of transport regulations.

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**15. REGULATORY INFORMATION**

Safety data sheets: according to Regulation (EC) No. 1907/2006

**Chemical Safety Assessment:**

A Chemical Safety Assessment has been carried out for this substance.

**INVENTORIES:**

EINECS: Conforms to  
TSCA: Conforms to  
AICS: Conforms to  
DSL: All components of this product are on the Canadian DSL list.  
ENCS (JP): Conforms to  
KECI (KR): Conforms to  
PICCS (PH): Conforms to  
IECSC (CN): Conforms to  
NZIOC: Does not conform  
TSCA 12B:

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**16. OTHER INFORMATION**

**Full text of R, H, EUH-phrases referred to under sections 2 and 3**

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.  
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.

Bibliography Fiche toxicologique INRS : N° 118 : ISOPHORONE

Further information When used in formulations, contact us for labelling.

**Update:**

Safety datasheet sections which have been updated:		Type:
1	Use of the Substance	Revisions
2	Classification and labelling, Potential health effects, Environmental Effects	Additions, Revisions
8	Derived No Effect Level (DNEL), Predicted No Effect Concentration (PNEC), Exposure controls	Additions
9	Boiling point/boiling range	Revisions
11	Aspiration hazard, Reproductive toxicity, Repeated dose toxicity	Additions
11	Acute toxicity, Eye contact, Specific Target Organ Toxicant, Carcinogenicity	Revisions
12	Aquatic toxicity, PBT assessment, Bioaccumulation, Distribution among environmental compartments, Henry constant, Surface tension	Revisions, Additions
15	Chemical Safety Assessment	Additions



**Thesaurus:**

NOAEL : No Observed Adverse Effect Level (NOAEL)  
LOAEL : Lowest Observed Adverse Effect Level (LOAEL)  
bw : Body weight  
food : oral feed  
dw : Dry weight  
vPvB : very Persistent and very Bioaccumulative  
PBT : Persistent, Bioaccumulative and Toxic

This information applies to the PRODUCT AS SUCH and conforming to specifications of TransChem. In case of formulations or mixtures, it is necessary to ascertain that a new danger will not appear. The information contained is based on our knowledge of the product, at the date of publishing and it is given quite sincerely. Users are advised of possible additional hazards when the product is used in applications for which it was not intended. This sheet shall only be used and reproduced for prevention and security purposes. The references to legislative, regulatory and codes of practice documents cannot be considered as exhaustive. It is the responsibility of the person receiving the product to refer to the totality of the official documents concerning the use, the possession and the handling of the product. It is also the responsibility of the handlers of the product to pass on to any subsequent persons who will come into contact with the product (usage, storage, cleaning of containers, other processes) the totality of the information contained within this safety data sheet and necessary for safety at work, the protection of health and the protection of environment.

**NB: In this document the numerical separator of the thousands is the "." (point), the decimal separator is "," (comma).**

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