



PRODUCT: ISOPHORONE (IS) REVISION:6

DATED: 05/05/11

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PRODUCT SPECIFICATION

Product Name:	Isophorone
Specification Reference	IS 440/447/5 (08/95)

SALES SPECIFICATION

PROPERTY	UNITS	VALUE	TEST
Purity	% mass	99.0 min	GC
Density	kg/l at 20°C	0.918 - 0.923	ASTM D4052-86
Water Content	% mass	0.10 max	BS 2511:1970 (1986) (using suitable Karl Fischer auto titrator)
Acidity	% mass as acetic acid	0.01 max	BS 553:1965 Appendix C modified
Appearance		Clear and free from matter in suspension	
Distillation range @ 1.013 bar			BS 4591:1971
Initial boiling point (BP)	°C	210 min	
dry point (DP)	°C	220 max	

PHYSICAL PROPERTIES

PROPERTY	CONDITIONS	UNIT	VALUE
Molecular mass			138.2
Density	20°C	kg/litre (vacuo)	0.9203
Relative density	20°C/20°C		0.9229
Change in relative density	20°C	per °C	0.78°10 ⁻³
Coefficient of Cubical expansion	20°C	per °C	0.85°10 ⁻³
Melting point		°C	-8.1
Boiling point	1.013 bar	°C	215.2
Change in boiling point	1.013 bar	°C/mbar	0.05
Vapour pressure	20°C	mbar	0.4
Flammable limits			
Upper	20 °C	% volume	3.8
Lower	20 °C	% volume	0.8
Flash point	Pensky Martens closed cup	°C	96
Auto ignition temperature	20°C	°C	462
Specific heat (liquid)	at boiling point	kJ/kg°C	1.78
Latent heat (of vaporisation)		kJ/kg	561
Critical temperature		°C	445
Critical pressure		bar	27.8
Critical volume	20°C	litres/kmole	470.0
Volume Resistivity	20°C	ohm.m	4.0°10 ⁴
Refractive Index		n ²⁰ _D	1.4781
Absolute viscosity	20°C	cP	2.62
Solubility			
in water	20°C	g/kg	12
water in solvent	20°C	g/kg	43
Evaporation rate	20°C		0.03
Relative to n-BuAc = 1			



NOTES

Exclusion of Liability

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Health and Safety

A Material Safety Data Sheet has been issued describing the health, safety and environmental properties of this product, identifying the potential hazards and giving advice on the handling precautions and emergency procedures. This must be consulted fully before handling, storage and use.



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SAFETY DATA SHEET

1. IDENTIFICATION OF THE SUBSTANCE/PREPARATION AND COMPANY

1.1 Product Identifier

Chemical Name (EINECS)	ISOPHORONE
CAS Number	78-59-1
EINECS Number	201-126-0
REACH Registration Number	01-2119497282-32-XXXX

1.2 Relevant identified uses of the substance or mixture

Industrial uses: Uses of substances as such or in preparation at industrial sites, formulation(mixing) of preparations/and/or re-packaging(excluding alloys), Professional uses: Public domain (administration, education, entertainment, services, craftsmen)

Solvent, Coatings and paints, thinners, paint removers, washing and cleaning products (including solvent based products), Intermediate, laboratory chemicals.

1.3 Details of the supplier of the safety data sheet

Tennants Distribution Limited
Hazelbottom Road
Cheetham
Manchester
M8 0GR
Tel: 44(0)161 205 4454
Fax: 44(0) 161 203 4298
Email: msds@tennantsdistribution.com

1.4 Emergency telephone number

Tel: 44(0)844 335 0001 (24 hours)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

2.1.1 Regulation 1272/2008 (CLP)

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

2.1.2 EEC Directive 67/548/EEC & Directive 1999/45/EC

Carc. Cat. 3; R40

Xn; R21/22

Xi; R36/37

Additional information; for full text of the R,H, EUH-phrases mentioned in this section , see Section 16.

2.2 Label elements

2.2.1

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

According to Regulation (EC) No. 1272/2008 (CLP).

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



Signal word(s) Warning.

Hazard statement(s)

Suspected of causing cancer.

Harmful if swallowed

Harmful in contact with skin.

Causes serious eye irritation.

May cause respiratory irritation.

Precautionary statement(s)

Prevention:

Do not handle until all safety precautions have been read and understood. P202

Avoid breathing gas/mist/vapours/spray. P261

Use personal protective equipment as required P281

Response:

If exposed or concerned: get medical advice/attention. P303+313



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Storage:

Store in a well-ventilated place. Keep container tightly closed. P403+233

2.3 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 to 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

Substances

- ISOPHORONE

CAS Number	EINECS Number	REACH registration number	Classification according to Directive 67/548/EEC	Classification according to Regulation 1272/2008	Concentration
78-59-1	201-126-0	01-2119497282-32-XXXX	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	>= 98.5%

See section 16 for the full text of the R, H- and EUH-phrases declared above

Occupational exposure limits, if available, are listed in section 8

4. FIRST AID MEASURES

4.1 Description of first aid measures

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 problem: Hospitalise.

Skin contact

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

Eye contact

Wash well-opened 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.

4.2 Most import symptoms and effects, both acute and delayed

Risks: No information available

4.3 Indication of any immediate medical attention and special treatment needed

For specialist advice physicians should contact the Poisons Information Service

5. FIRE FIGHTING MEASURES

5.1 Extinguishing Media

Suitable extinguishing media: Water spray, carbon dioxide (CO₂), foam, dry powder.

Unsuitable extinguishing media: high volume water jet.

5.2 Special hazards arising from the substance or mixture

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

5.3 Advice for fire-fighters

Specific methods:

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

Specific protective actions for fire-fighters:

Wear self contained breathing apparatus and protective suit.



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6. ACCIDENTAL RELEASE MEASURES

6.1 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.

6.2 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).

6.3 Methods and material for containment and cleaning up

Recovery:

Place in suitable container. Absorb the remainder with an inert absorbent material. After cleaning, flush away traces with water. Recover waste 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 and waste water

7. HANDLING AND STORAGE

7.1 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 point of use.

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 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

7.2 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 oxidising agents, strong bases

Packing material:

Recommended: Steel

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

7.3 Specific end use(s)

None

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Exposure Limit values

Isophorone

Source	Date	Value type	Value (ppm)	Value (mg/m ³)	Remarks
EH40 WEL	2007	STEL	5	29	-
ACGIH(US)	2007	Ceiling	5	-	-

Derived No Effect Level (DNEL):

End Use	Inhalation	Ingestion	Skin Contact
Workers	22 mg/m ³ (ST,SE,LE) 11 mg/m ³ (LT,SE,LE)		41 mg/kg bw/day (ST,SE) 20.5 mg/kg bw/day (LT,SE)

LE: Local effects, SE: Systematic effects, LT: long term, ST: short term

Predicted No Effect Concentrations (PNEC):

Compartment:	Value:
Water	0.089mg/l
Marine water	0.0089mg/l
Water (intermittent release)	1.2mg/l
Effects on waste water treatment plants	1mg/l
Sediment	0.839mg/kg dw
Marine sediment	0.0839 mg/kg dw



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Soil	0.12mg/kg dw
Oral (secondary poisoning)	0.02 mg/kg food
8.2 Exposure controls	
General protective measures	
Ensure sufficient air exchange and/or exhaust in work areas	
Respiratory protection	
If vapour present use suitable respiratory protection checking filter is suitable for Isophorone	
Hand protection	
PVC gloves	
According to permeation index EN 374:1 (time elapsed > 10 mins)	
Eye protection	
Safety glasses	
Skin protection	
At the workplace: Protective clothing	
Intervention at incident: Protective clothing	
Environmental exposure controls	
See chapter 6	
9. PHYSICAL AND CHEMICAL PROPERTIES	
9.1 Information on basic physical and chemical properties	
Appearance	
Physical State (20°C)	Liquid
Colour	Light yellow
Odour	Smelling of camphor
Olfactory threshold	0.2ppm
pH in water solution	No data available
Melting point/range	-8.1°C
Formation of azeotrope with water	
Boiling point/boiling range	215.3°C (pressure 1,013 hPa)
Flash point	Closed cup: 80-85°C (standard NF 60 103)
Evaporation rate	No data available
Flammability (solid, gas)	
Lower flammability limit	0.8% (V)
Higher flammability limit	3.8% (V)
Vapour pressure	0.4 hPa, at 20°C
Vapour density	5.7 kg/m ³
Density	920 kg/m ³ , at 20°C
Relative density (Water=1)	0.92 at 20°C
Water solubility	12 g/l
	40g/l Solubility of water in the product
Partition coefficient: N-octanol/water	Log Kow: 1.67, at 20°C (OECD Guideline 107)
Auto ignition temperature	462°C (Standard BS 4056 1966)
Decomposition temperature	No data available
Viscosity dynamic	2.62 mPa.s, at 20°C
9.2 Explosive properties	
Explosivity	Not relevant (due to chemical structure)
Oxidizing properties	Not relevant (due to chemical structure)
9.2 Other information	
Solubility in other solvents	Soluble in most organic solvents
Surface tension	32.3mN/m Surface tension
Henry constant	380E-03 Pa.m ³ /mol
Molecular weight	138.2g/mol
Refractive index	1.476 at 20°C
10. STABILITY AND REACTIVITY	
10.1 Reactivity	
No data available	
10.2 Conditions to avoid	
Keep away from heat and sources of ignition	



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10.3 Incompatible materials

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

10.4 Hazardous decomposition products

Thermal decomposition giving toxic products, Carbon Monoxide

10.5 Further Information

The product is stable under normal handling and storage conditions.

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.

11.1 Information on toxicological effects

Components: Isophorone

Inhalation Toxicity

Slightly harmful by inhalation

In man: At high vapour /mist concentrations, Risk of headache, drowsiness, narcosis, suffocation

In animals:LC50/4/rat: 7mg/l (aerosol)

Acute Oral Toxicity

Harmful if swallowed

In animals:LD50/rat: 1,500-3,450 mg/kg

Acute Dermal Toxicity

Harmful if in contact with the skin

In animals:LD50/rat:1,700 mg/kg

Skin Corrosion/Irritation

In animals: Mild skin irritation (OECD Guidelines 404, rabbit, exposure time 4h)

Serious eye damage/eye irritation

In man: Exposure to vapours, eye irritation (0.37mg/l)

In animals: Eye irritation (Draize Test , rabbit)

11.2 Information on respiratory or skin sensitisation

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)

11.3 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)(2years, 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 reproductive system, NOAEL: 1000mg/kg (rat, mouse ,By oral route, 3 months)

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: 0.66mg/l

Maternal concentration without effect: 0.29mg/l (Method: OECD Test Guideline414, rat, mouse, By inhalation)



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11.4 Specific Target Organ Toxicity

Single Exposure

Irritating to respiratory system

Exposure routes: inhalation

Target Organs: upper respiratory tract

Inhalation

Olfactory threshold:0.2ppm

In man: exposure to vapours

Irritation (throat) (0.20 mg/l)

Irritation to nasal mucous membranes (0.37 mg/l)

Repeated Exposure

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

In animals: By inhalation: concentration has no effect on nasal mucous membranes

> 0.51mg/l (mouse, 2 weeks)

By oral route: No specific toxic effects

NOAEL= >233mg/kg bw/day (rat, 13 weeks)

Aspiration Hazard

Not applicable

12. ECOLOGICAL INFORMATION

12.1 Acute Toxicity

Fish:

Practically non-toxic.

LC50 ,96 h (Pimephales promelas (fathead minnow)) : 228mg/l (test substance: active ingredient)

Aquatic Invertebrates:

Practically non toxic

EC(I) 50, 8h (Daphnia magna (Water flea)) : 120mg/l (Method : US EPA< Immobilisation, Test substance: Active ingredient)

Aquatic plants:

Practically non toxic

IC50, 72 h (Desmodesmus subspicatus (green algae)): 475.4 mg/l (test substance: active ingredient) NOEC :64 mg/l

Micro organisms:

Practically non toxic

EC10, 18h (Pseudomonas putida): 328 mg/l (Method : no data available, Growth inhibition, test substance. Active ingredient)

EC50, 3h (Activated sludge): 100 mg/l (Method: OECD Guideline 209, Respiration inhibition, Test substance: Active ingredient)

12.2 Aquatic toxicity/ Long term toxicity:

Fish

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

Lowest observed concentration: 19mg/l

12.3 Persistence and degradability

Biodegradation (in water):

Readily biodegradable

95% after 28 d (Method :OECD Guideline 301 A)

12.4 Bio accumulative potential

Does not bioaccumulate

Partition coefficient: N-octanol/water: log Kow: 1.67, at 20°C (Method: OECD Guideline 107)

Bioconcentration factor (BCF) :1.1-1.8 (42d, Method: OECD Guideline 305C, Cyprinus carpio (Carp), Test substance: Active ingredient) Fish

12.5 Mobility in soil

Distribution among Water: 87.6%

Environmental compartment: Air:11.7% (method :Calculation according Mackay, Level1)

Henry constant: 380E-03 Pa.m3/mol

Surface tension: 32.3 mN/m Surface tension

Absorption/desorption: Non adsorbable (Method: calculated)

12.6 Results of PBT and vPvB assessment

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

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

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.

15. REGULATORY INFORMATION

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

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

UK REGULATION : Chips3 : Chemical (Hazard Information and Packaging for Supply) Regulations 2002

15.2 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:ENCS (JP):

All components of this product are on the Canadian DSL list.

KECI (KR):

Conforms to

PICCS (PH):

Conforms to

IECSC (CN):

Conforms to

16. OTHER INFORMATION

Full text of R 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

Full text of H-Statements referred to under sections 2 and 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.

Source of key data used to compile the data sheet

Bibliography: Fiche toxicologique INRS :no 118 : Isophorone

Modifications from last revision

The Safety Data Sheets have been revised throughout to conform to EC Directive 1907/2006 and amendments

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