GPS Safety Summary

Substance Name:

3,5,5-trimethylcyclohex-2-enone

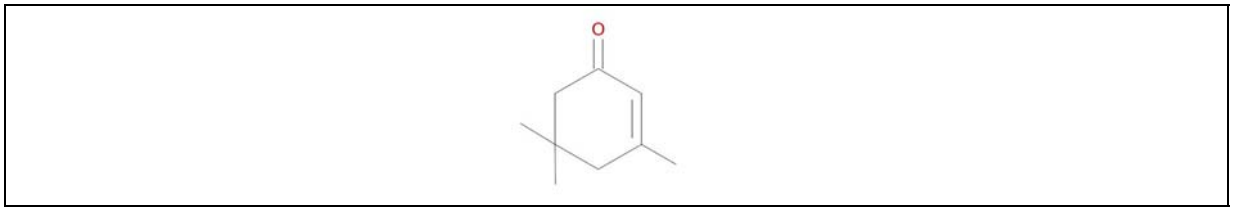
1. General Statement

3,5,5-trimethylcyclohex-2-enone is a light yellow liquid highly soluble in water. It is an oxygenated solvent commonly named Isophorone (IPHO).

IPHO is manufactured, used and formulated within industrial and professional settings. This substance is also present in some specific preparations used by consumers.

2. Chemical Identity

Name:	3,5,5-trimethylcyclohex-2-enone
Brand names:	IPHO
Chemical name (IUPAC):	3,5,5-Trimethyl-2-cyclohexene-1-one
CAS number(s):	78-59-1
EC number:	201-126-0
Molecular formula:	$C_9H_{14}O$
Structure:	



3. Use and applications

The major use of 3,5,5-trimethylcyclohex-2-enone is as an intermediate and as a solvent in the coatings, cleaning and agrochemical industries.

- Synthesis of IPDA and IPDI: (isophorone diamine and isophorone diisocyanate) used in the manufacturing of epoxy, isocyanate and polyamide resins.
- Chemical synthesis: 3,5-xylenol, TMCHONE and TMCHOL (synthetic menthol) synthesis.
- Pharmaceuticals: Synthesis of Active Ingredients: Cyclonicate, Cyclandelate, Homosalate, Neramexane.
- Agrochemicals: Miscellaneous herbicide and insecticide formulations,
- Paints and varnishes: Excellent solvent for PVDF resins. Levelling aid for polyacrylate, alkyde, epoxy, urea-formaldehyde, phenolic resins. Gloss properties.

4. Physical / Chemical properties

3,5,5-trimethylcyclohex-2-enone is a liquid organic substance having the following characteristics and physico–chemical properties:

Property	Value
Physical state	liquid at 20°C and 1013 hPa
Colour	light yellow
Odour	smelling of camphor
Molecular weight	138.21 g/mol
Density	0.920 at 20°C
Vapour pressure	0.4 hPa at 20°C
Freezing / boiling points	-8.1°C / 215.3°C at 1013hPa
Flammability	Flammable when hot
Flash point	80 - 85°C (closed cup)
Self-ignition temperature	462°C at 1013 hPa
Explosive / oxidizing properties	Not relevant based on its structure
Water solubility	12 g/L at 20°C (highly soluble at 20°C) 40 g/L solubility of water in the product
Dissociation constant (pK_a)	Not relevant based on its structure
Octanol-water partition coefficient (Log K_{ow})	1.67 at 20°C

5. Health Effects

Effect Assessment	Result
Acute Toxicity Oral / inhalation / dermal	Harmful by ingestion and dermal contact and of low toxicity by inhalation exposure
Irritation / corrosion Skin / eye/ respiratory tract	Slightly irritating to the skin and irritating to the eyes and the respiratory tract
Sensitisation	Not sensitising
Toxicity after repeated exposure Oral / inhalation / dermal	Repeated exposures by inhalation induce an irritation of the respiratory tract in laboratory animals. No significant systemic toxicity following repeated oral administration
Genotoxicity / Mutagenicity	Not genotoxic
Carcinogenicity	Limited evidence for a carcinogenic effect
Reproductive / Developmental Toxicology	No effects were observed on fertility and foetal development in treated laboratory rats.

6. Environmental Effects

The potential of 3,5,5-trimethylcyclohex-2-enone for bioaccumulation is low. This product will not persist in the environment. It is slightly harmful to aquatic organisms.

Effect Assessment	Result
Aquatic Toxicity	Slightly harmful to aquatic organisms

Fate and behaviour	Result
Biodegradation	Readily biodegradable
Bioaccumulation potential	Not expected to bioaccumulate
PBT / vPvB conclusion	Not considered as PBT* or vPvB**

*: Persistent, Bioaccumulative and Toxic (PBT)
**: very Persistent and very Bioaccumulative (vPvB)

7. Exposure

7.1 Human health

3,5,5-trimethylcyclohex-2-enone (IPHO) is manufactured, used and formulated within industrial and professional settings.

The primary routes of industrial exposure of IPHO are skin contact and inhalation, ingestion is not an anticipated route of exposure. Workers may be exposed during cleaning, maintenance, transfer, sampling and analysis.

Based on the risk assessment, the exposure can be kept at a safe level (strictly below occupational exposure limits, when applied) when activities are carried out under conditions recommended in the Extended Safety Data Sheet (see Chap. 8 and Exposure Scenarios).

Procedures, controls, suitable collective and personal risk management measures, good industrial hygiene practices and risk and communication through appropriate training of workers should be implemented.

In case of exposure to the undiluted substance, workers should follow the first aid measures recommended in the Safety Data Sheet.

7.2 Environment

The assessment of the environmental exposure is made for all the uses and resulted life cycle stages of the substance from the manufacture to the waste stage.

IPHO is manufactured and used in continuous or batch processes within industrial settings.

Based on the risk assessment, environmental exposure can be kept at a safe level when activities are carried out under conditions recommended in the extended Safety Data Sheet (see Chap. 6, and Exposure Scenarios).

All industrial aqueous releases that may contain the substance must be treated to avoid any exposure to the environment.

Disposal, treatment or recycling of industrial waste must comply with applicable regulations to preserve the environment.

Procedures, controls and risk management measures should be implemented on industrial manufacturing and application sites; effluents that may contain the substance must be treated to avoid any exposure to the environment.

8. Risk Management recommendations

Human health measures		
Organizational	Collect the latest available Safety Data Sheet. Implement good basic standards of occupational health. Ensure operatives are well informed of the hazards and trained to minimise exposures. Handle and store according to the indications of the Safety Data Sheet.	
Engineering controls	Provide appropriate local exhaust ventilation at points of emission. Ensure that eye- and handwash stations and safety showers are close to workstation locations.	
Protection	**Eye/Face protection:**	Safety glasses with side-shields
	Skin and body protection:	At the workplace: Protective clothing (cotton) Intervention at incident: Waterproof suit
	Hand protection:	Gloves (Polyvinylchloride), tested to EN374:1
	Respiratory protection:	Low concentrations or short activity: Mask with specific cartridge. Recommended Filter type: A High concentrations or prolonged activity: Self contained Breathing Apparatus
Environment protective measures		
Do not release into the environment. Do not let product enter drains. Use waste water treatment systems. Do not spread sludge to soil. Elimination: Destroy the product by incineration (in accordance with local and national regulations) (see chap. 6 of the Safety Data Sheet).		

9. Regulatory Information / Classification and Labelling

9.1 Regulatory Information

This substance has been registered under:

- EU Regulation EC 1907/2006 (REACH)

9.2 Classification and labelling

Under GHS substances are classified according to their physical, health, and environmental hazards. The hazards are communicated via specific labels and the eSDS. GHS attempts to standardize hazard communication so that the intended audience (workers, consumers, transport workers, and emergency responders) can better understand the hazards of the chemicals in use. Substances registered for REACH are classified according to CLP (EC) 1272/2008, implementation of the GHS in the European Union.

Classification
According to REGULATION (EC) no 1272/2008: - Acute toxicity – Oral: Category 4 - Acute toxicity – Dermal: Category 4 - Eye irritation: Category 2 - Specific target organ toxicity - single exposure (inhalation): Category 3 - Carcinogenicity: Category 2

Signal word	
— Warning	
Pictogram	
— GHS08: health hazard	
— GHS07: exclamation mark	
Hazard statement	
— 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	
Alternative classification according to Globally Harmonized System (GHS)	
— Flammable liquids: Category 4, H227: Combustible liquid. — Acute toxicity – Oral: Category 4, H302: Harmful if swallowed. — Acute toxicity – Dermal: Category 4, H312: Harmful in contact with skin. — Acute toxicity – Inhalation: Category 5, H333: May be harmful if inhaled. — Eye irritation: Category 2A, H319: Causes serious eye irritation. — Specific target organ toxicity - single exposure (inhalation): Category 3, H335: May cause respiratory irritation. — Carcinogenicity: Category 2, H351: Suspected of causing cancer.	

10. Contact Information within Company

For further information on this substance or product safety summary in general, please contact:

— arkema-thio-reach-uses@arkema.com

— **ICCA portal where the GPS Safety Summary is posted**: http://www.icca-chem.org/en/Home/ICCA-initiatives/global-product-strategy/

11. Date of Issues / Revision

— Date of issue: 2014/10/31

— Date of revision:

12. Disclaimer

The information contained in this paper is intended as advice only and whilst the information is provided in utmost good faith and has been based on the best information currently available, is to be relied upon at the user's own risk.

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