November 2015

Properties, Hazards and Safety Information for IPDI*

Product: IPDI (Isophorone diisocyanate; CAS No. 4098-71-9)

Physical and chemical data

Physical state	liquid
Colour	colourless to yellowish
Odour	pungent
Melting point/range	-60°C
Boiling point/range	310 °C (1013 hPa)
Flash point	150.5 °C (1013 hPa)
Self-ignition temperature	430°C
Lower/upper explosion limit	0.7/4.5% (Vol.)
Vapour pressure	0.000635 hPa at 20 °C 0.00117 hPa at 25 °C 0.0212 hPa at 50 °C
Density	1.06 g/cm3 (20°C)
Water solubility	approx. 15 mg/l (23°C)
Viscosity	approx. 10mPas (25°C)
Thermal decomposition	Beginning at approximately 260 °C.
Hazardous decomposition products	no dangerous decomposition products if properly stored and handled
Hazardous reactions	with amines, acids, bases, strong oxidants, alcohols. Decomposes in water with formation of CO_2 (leading to an increase in pressure in closed containers!)

***More detailed information should be taken from the suppliers' Material Safety Data Sheets**

Toxicological Information

Short term exposure

Ingestion	Acute oral toxicity is low: LD_{50} (rat) = 4,814mg/kg bw Ingestion may irritate the gastro-intestinal tract.
Skin contact	Acute dermal toxicity is low: LD_{50} (rat) > 7,000 mg/kg IPDI is corrosive to skin. The substance is a skin sensitizer.
Eye contact	IPDI causes serious eye damage.
Inhalation	IPDI is very toxic by inhalation of aerosols (LC50, rat = 0.031 mg/l/4h). Vapour and aerosols are severely irritating to the respiratory tract. High exposure can result in inflammation of lung tissue and fluid in the lungs. In sensitized people very low concentrations may lead to asthmatic symptoms, the onset of which may be delayed for several hours.

Repeated exposure / longterm effects

Skin contact	May cause sensitization by skin contact.
Inhalation	May cause sensitization by inhalation. Chronic exposure by inhalation may result in permanent decrease in lung function.
Genotoxicity	Based on studies conducted with bacteria, mammalian cell cultures and animals IPDI showed no genotoxicity with relevance to men.
Carcinogenicity	No animal studies have been performed yet.
Reproductive toxicity	In a developmental toxicity study with exposure by inhalation, no developmental toxicity was observed in the absence of maternal toxicity.

Exposure controls/Personal protection equipment

General	Workers with a hypersensitivity of the respiratory tract and/or the skin (e.g. asthmatics or those suffering from chronic bronchitis or chronic skin complaint) should not be exposed to this chemical.
OELs	In many countries occupational exposure limits for IPDI have been set up. These can be found under →OELs IPDI (see website under Library – Regulatory Information)

DNEL

Application Area	Workers	Workers
Route of Exposure	Inhalation	Inhalation
Health Effect	Acute - local effects	Long-term - local effects
mg/m3	0.0453 mg/m3	0.0453 mg/m3

PNEC

$PNEC_{freshwater}$	$PNEC_{marine\ water}$	$PNEC_{STP}$	$PNEC_{sediment\ freshwater}$	$PNEC_{sediment\ marine\ water}$	$PNEC_{soil}$
0.06 mg/L	0,006 mg//L	0.04 mg/L	218.92 mg/Kg dw	21.89 mg/kg dw	44.01 mg/kg dw

Respiratory protection	Respiratory protection is required if an inhalative expsorue can not be excluded. Depending on the exposure scenario relevant for the interesting application more details are given in the extended MSDS of the supplier.
Hand protection	Chemical resistant protective gloves should be worn, e.g. - butyl rubber with a thickness ≥ 0.5 mm (breakthrough time ≥ 480 min) - fluorinated rubber with a thickness ≥ 0.4 mm (breakthrough time ≥ 480 min) - nitrile rubber with a thickness ≥ 0.35 mm (breakthrough time ≥ 480 min) - polyvinyl chloride with a thickness ≥ 0.5 mm (breakthrough time ≥ 480 min) Contaminated gloves should be disposed of.
Body protection	Body protection should be chosen based on activity and possible exposure, e.g. apron, protecting boots, chemical-protection suit.
Eye protection	Face protection/close-fitting protective goggles should be worn.

First aid measures

General	Contaminated clothing must be taken off immediately.
Skin contact	Remove any contaminated clothing immediately. Wipe off mechanically and wash affected areas thoroughly with soap and water for at least 15 minutes. Dispose of contaminated clothing or was thoroughly before reuse. For severe exposures, the affected person should get under a safety shower, using the flushing action of the water to remove the bulk of the chemical, then remove contaminated clothing and wash skin with soap and water. Seek medical attention. For lesser exposures, the individual should seek medical attention if irritation develops or persists after the area is washed.
Inhalation	The person should move to an area free from risk of further exposure. Oxygen or artificial respiration should be administered as needed. Asthmatic-type symptoms may develop and may be immediate or delayed up to several hours.

	Treatment is essentially symptomatic. A physician should be consulted.
Eye contact	Flush with large amounts of lukewarm water for at least 15 minutes, holding eyelids open all the time. Refer the affected individual to an eye specialist or other physician for immediate follow-up.
Ingestion	Vomiting should not be induced and nothing should be given orally to an unconscious or convulsing person. A physician should be consulted.

Ecological information

Biodegradability	IPDI is not readily biodegradable. It reacts with water forming solid insoluble polyurea, isophorone diamine (IPDA) and CO_2, thus the predominant removal mechanism is expected to be hydrolysis. IPDA is not readily biodegradable. However, in a simulation test with activated, non-adapted sludge, a degradation of 42 % was measured after a contact time of 6 hrs.
Bioaccumulation	Due to hydrolysis in water bioaccumulation of IPDI is not expected. The bioaccumulation potential of the hydrolysis product IPDA is considered to be low (log K_{ow} = 0.99).
Acute toxicity to aquatic organisms	IPDI reveals a moderate level of aquatic toxicity: - LC50 (fish, *Brachydanio rerio*, 96h) > 72.3mg/l - LC50 (fish, *Cyprinus carpio*, 96h) > 208 mg/l - EC50 (bacteria, 3h) = 263 mg/l - EC50 (*Daphnia magna*, 48h) = 27 mg/l - ErC50 (algae, *Scenedesmus subspicatus*, 72h) 70 mg/l - NOEC (algae, *Scenedesmus subspicatus*, 72h) 4.4 mg/l The hydrolysis product IPDA was observed to be toxic to aquatic organisms: - LC50 (fish, *Leuciscus idus*, 96h) 110 mg/l - EC50 (bacteria, *Pseudomonas putida*, 18h) = 1120 mg/l - EC50 (*Daphnia magna*, 48h) = 23 mg/l - NOEC (*Daphnia magna*, 21d) = 3.0 mg/l - ErC50 (algae, *Scenedesmus subspicatus*, 72h) >50 mg/l

EC Classification and labeling

A) According CLP regulation 1272/2008

1.1 Classification according Annex VI, Table 3.1 (legally binding)

hazard class	category	hazard phrase
acute inhalative toxicity	1	H330: Fatal if inhaled
skin corrosion/irritation	2	H315: Causes skin irritation
eye irritation	2	H319: Causes serious eye irritation
respiratory sensitisation	1	H334: May cause allergy or asthma symptoms or breathing difficulties if inhaled
skin sensitisation	1	H317: May cause an allergic skin reaction
STOT SE	3	H335: May cause respiratory irritation
hazardous to aquatic environment	chronic 2	H411: Toxic to aquatic life with long lasting effects

1.2 Self classification (based on available data)

hazard class	category	hazard phrase
acute inhalative toxicity	1	H330:Fatal if inhaled
skin corrosion/irritation	1C	H314: Causes severe skin burns and eye damage
respiratory sensitisation	1	H334: May cause allergy or asthma symptoms or breathing difficulties if inhaled
skin sensitisation	1	H317: May cause an allergic skin reaction

2. Labeling according regulation 1272/2008 (CLP)

2.1 According Annex VI, Table 3.1 (legally binding)

Pictograms	
Signal word	Danger
Hazard statement	H330:Fatal if inhaled
	H319: Causes serious eye irritation H335: May cause respiratory irritation H315: Causes skin irritation
	H334: May cause allergy or asthma symptoms or breathing difficulties if inhaled
	H317: May cause an allergic skin reaction
	H411: Toxic to aquatic life with long lasting effects

2.2 Based on Self Classification (based on available data)

Pictograms	
Signal word	Danger
Hazard statement	H330:Fatal if inhaled
	H314: Causes severe skin burns and eye damage
	H334: May cause allergy or asthma symptoms or breathing difficulties if inhaled

B.) Classification and labeling according Annex VI, Table 3.2 of regulation 1272/2008 (CLP)

Symbols	T N	Toxic Dangerous for the environment
Risk phrases	R23 R36/37/38 R51/53	Toxic by inhalation Irritating to eyes, respiratory system and skin Toxic to aquatic organisms. May cause long-term adverse effects in the aquatic environment.
Safety phrases	S26 S28 S38 S45	In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. After contact with skin, wash immediately with plenty of soap and water. In case of insufficient ventilation, wear suitable respiratory equipment. In case of accident of if you feel unwell, seek medical advice immediately (show the label where possible).