

Safety Data Sheet

Isophorone diisocyanate

Version : V2.0.0.1

Report No. : BWJ5448-2016-MSDS-EP

Creation Date : 2026/01/16

Revision Date : -



*Prepared in accordance with EU REACH Regulation (REACH 1907/2006 with amendment 2020/878)

1 Identification of the substance/mixture and of the company/undertaking

1.1 Product identifier

Product Name	Isophorone diisocyanate
Cat No.	BWJ5448-2016
CAS No.	4098-71-9
EC No.	223-861-6
Molecular Formula	C ₁₂ H ₁₈ N ₂ O ₂
REACH Registration Number	-
UFI	Not applicable

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

Relevant identified uses	Please consult manufacturer.
Uses advised against	Please consult manufacturer.

1.3 Details of the supplier of the Safety Data Sheet

Name of the company	Weiyel Inc
Address of the company	Hedian Light Industrial Park, Chengguan Town, Shangcheng County, Xinyang City, Henan Province, China
Post code	465350
Telephone number	010-58103678
Fax number	010-84840368
E-mail address	info@weiyel.com

1.4 Emergency telephone number

Emergency telephone number	010-58103678
Opening hours	24h

2 Hazards identification

2.1 CLP classification according to Regulation (EC) No. 1272/2008 with amendment 2023/707

Skin Corrosion/Irritation	Category 2
Sensitization - skin	Category 1
Serious eye damage/irritation	Category 2
Acute Toxicity - Inhalation	Category 1
Sensitization - respiratory	Category 1
Specific target organ toxicity -	Category 3

single exposure; respiratory tract irritation	
Hazardous to the aquatic environment - long-term (chronic) hazard	Category 2

2.2 Label elements

Hazard pictograms	
Signal word	Danger

Hazard statements

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

Precautionary statements

◆ Prevention

P260	Do not breathe dust/fume.
P264	Wash hands and other parts of the body (if related) thoroughly after handling.
P271	Use only outdoors or in a well-ventilated area.
P272	Contaminated work clothing should not be allowed out of the workplace.
P273	Avoid release to the environment.
P280	Wear protective gloves/protective clothing/eye protection/face protection.
P284	[In case of inadequate ventilation] wear respiratory protection.

◆ Response

P310	Immediately call a POISON CENTER/doctor.
P320	Specific treatment is urgent (see related instructions on the label).
P321	Specific treatment (see related instructions on the label).
P391	Collect spillage.
P302+P352	IF ON SKIN: Wash with plenty of water.
P304+P340	IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P333+P313	If skin irritation or rash occurs: Get medical advice/attention.
P337+P313	If eye irritation persists: Get medical advice/attention.
P342+P311	If experiencing respiratory symptoms: Call a POISON CENTER/doctor.
P362+P364	Take off contaminated clothing and wash it before reuse.
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

◆ Storage

P405	Store locked up.
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P403+P233

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

◆ Disposal

P501

Dispose of contents/container in accordance with local/regional/national/international regulations.

2.3 Other hazards

◆ Results of PBT and vPvB assessment

Component	Results of PBT and vPvB assessment [according to (EC) No 1907/2006]
3-isocyanatomethyl-3,5,5-t rimethylcyclohexyl isocyanate	Not PBT/vPvB

◆ Results of endocrine disrupting properties assessment

Component	Results of endocrine disrupting properties assessment [according to (EU) No 2017/2100 or (EU) No 2018/605]
3-isocyanatomethyl-3,5,5-t rimethylcyclohexyl isocyanate	Insufficient information, temporarily unable to evaluate

◆ Other

Not applicable.

3 Composition/information on ingredients**3.1 Substance**

Component	Weight % content(or range)	Classification according to Regulation (EC) No. 1272/2008 with amendment 2023/707 [CLP]	Specific Conc. Limits, M-factors
3-isocyanatomethyl-3,5,5- -trimethylcyclohexyl isocyanate CAS : 4098-71-9 EC : 223-861-6 Index No. : 615-008-00-5	99.89	Skin Corrosion/Irritation, Category 2, H315; Sensitization - skin, Category 1, H317; Serious eye damage/irritation, Category 2, H319; Acute Toxicity - Inhalation, Category 3, H331; Sensitization - respiratory, Category 1, H334; Specific target organ toxicity - single exposure; respiratory tract irritation, Category 3, H335; Hazardous to the aquatic environment - long-term (chronic) hazard, Category 2, H411	H334:C ≥ 0.5% H317:C ≥ 0.5%

3.2 Mixture

Not applicable

4 First-aid measures**4.1 Description of first aid measures**

General advice	Immediate medical attention is required. Show this safety data sheet (SDS) to the doctor in attendance.
Eye contact	Rinse with plenty of water (remove contact lenses if easily possible). Refer immediately for medical attention.
Skin contact	Remove contaminated clothes. Rinse and then wash skin with water and soap. Refer for medical attention.

Ingestion	Rinse mouth. Do NOT induce vomiting. Give one or two glasses of water to drink. Refer for medical attention.
Inhalation	Fresh air, rest. Half-upright position. Refer immediately for medical attention.
Protecting of first-aiders	Ensure that medical personnel are aware of the substance involved. Take precautions to protect themselves and prevent spread of contamination.

4.2 Most important symptoms/effects, acute and delayed

1	Substance accumulation, in the human body, may occur and may cause some concern following repeated or long-term occupational exposure.
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4.3 Indication of any immediate medical attention and special treatment needed

1	Treat symptomatically.
2	Symptoms may be delayed.

5 Fire-fighting measures

5.1 Extinguishing media

Suitable extinguishing media	Small fire: CO ₂ , dry chemical, dry sand, alcohol-resistant foam; Large fire: water spray, fog or alcohol-resistant foam; Fire involving tanks, rail tank cars or highway tanks: Fight fire from maximum distance or use unmanned master stream devices or monitor nozzles. Cool containers with flooding quantities of water until well after fire is out. Do not get water inside containers.
Unsuitable extinguishing media	Large fire: avoid aiming straight or solid streams directly onto the product.

5.2 Specific hazards arising from the substance or mixture

1	May emit poisonous fumes on fire.
2	Development of hazardous combustion gases or vapor possible in the event of fire.
3	May expansion or decompose explosively when heated or involved in fire.

5.3 Advice for firefighters

1	As in any fire, wear self-contained breathing apparatus (MSHA/NIOSH approved or equivalent) and full protective gear.
2	Fight fire from a safe distance, with adequate cover.
3	Prevent fire extinguishing water from contaminating surface water or the ground water system.

6 Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

1	Fully encapsulating, vapor protective clothing should be worn for spills and leaks with no fire.
2	Do not touch or walk through spilled material.
3	Do not touch damaged containers or spilled material unless wearing appropriate protective clothing.
4	Ensure adequate ventilation. Remove all sources of ignition. Take precautionary measures against static discharges.
5	Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.
6	Use personal protective equipment, do not breathe dust/fume.

6.2 Environmental precautions

1	Prevent further leakage or spillage if safe to do so.
2	Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

1	Isolation of contaminated areas and restrictions on access.
2	It is recommended that emergency personnel wear dust masks and wear anti-virus suits.
3	Do not touch broken containers and spills before putting on appropriate protective clothing.
4	Cover the spill with a plastic sheet to reduce scattering.
5	Cut off the source of the leak as much as possible.
6	Keep leaks in a ventilated place.
7	It is recommended that emergency personnel wear dust masks.
8	Collect the spill with a clean shovel and place it in a clean, dry, loosely closed container and move the container away from the leak.
9	Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

6.4 Reference to other sections

1	Personal Protective Equipment advice is contained in Section 8 of the SDS.
2	Disposal considerations advice is contained in Section 13 of the SDS.

7 Handling and storage

7.1 Precautions for safe handling

◆ Protective measures

1	Handling is performed in a well ventilated place.
2	Wear suitable protective equipment.
3	Avoid contact with skin and eyes.

◆ Measures to prevent fire

1	Keep away from heat/sparks/open flames/ hot surfaces.
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◆ Measures to prevent aerosol and dust generation

1	Avoid formation of dust and aerosols.
2	Provide appropriate exhaust ventilation at places where dust is formed.

◆ Advice on general occupational hygiene

1	Wash hands and face after using the substances.
2	Replace the contaminated clothing immediately.

7.2 Conditions for safe storage, including any incompatibilities

1	Keep containers tightly closed.
2	Keep containers in a dry, cool and well-ventilated place.
3	Keep away from heat/sparks/open flames/hot surfaces.
4	Store away from incompatible materials and foodstuff containers.

7.3 Specific end use(s)

1	In addition to use mentioned in the Section 1.2, unforeseen other specific end uses.
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8 Exposure controls/personal protection

8.1 Control parameters

◆ Occupational exposure limit values

Component	Country/Region	Limit value - Eight hours		Limit value - Short term	
		ppm	mg/m ³	ppm	mg/m ³
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	Permissible exposure standards for workers in the workplace	0.005	0.045	0.015	0.135
	France	0.01	0.09	0.02	0.18
	Germany (AGS)	0.005	0.046	0.005	0.046
	Germany (DFG)	0.005	0.046	0.005	0.046
	Austria	0.01	0.09	0.02	0.18
	Belgium	0.005	0.046	-	-

◆ Biological limit values

Biological limit values	No relevant regulations
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◆ Monitoring methods

1	EN 14042 Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents.
2	GBZ/T 300 and GBZ/T 160 series standard Determination of toxic substances in workplace air.

◆ Derived No effect level (DNEL)

Component	Route of exposure	DNEL for Workers			
		Acute effects (local)	Acute effects (systemic)	Chronic effects (local)	Chronic effects (systemic)
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	Inhalation	No data available	No data available	0.045 mg/m ³	No data available
	Oral	No data available	No data available	No data available	No data available
	Dermal	No data available	No data available	No data available	No data available

◆ Predicted No Effect Concentration (PNEC)

Component	A	B	C	D	E	F	G	H
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	27 µg/L	400 ng/L	10.6 mg/L	98.51 mg/kg sediment dw	1.46 mg/kg sediment dw	No hazard identified	19.8 mg/kg soil dw	No potential for bioaccumulation

Note :

A: Freshwater; B: Seawater; C: Sewage treatment plant; D: Sediment (freshwater); E: Sediment (seawater); F: Air; G: Soil; H: Secondary poisoning(Hazard for Predators).

8.2 Exposure controls

8.2.1 Engineering controls

1	Ensure adequate ventilation, especially in confined areas.
2	Ensure that eyewash stations and safety showers are close to the workstation location.
3	Use explosion-proof electrical/ventilating/lighting/equipment.
4	Set up emergency exit and necessary risk-elimination area.

8.2.2 Personal protection equipment

General requirement	
Eye protection	Must wear appropriate safety goggles.
Hand protection	Must wear appropriate chemical protective gloves.
Respiratory protection	Must wear appropriate personal dust proof gas mask.
Skin and body protection	Must wear appropriate chemical protective clothing and chemical resistant shoes.

8.2.3 Environmental exposure controls

Environmental exposure controls	No information available
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9 Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state	white or light yellow solid powder
Colour	white or light yellow solid powder
Odor	No information available
Odor threshold	No information available
pH	No information available
Melting point/freezing point(°C)	-60
Initial boiling point and boiling range(°C)	158 (1.33kPa)
Flash point(Closed cup,°C)	155
Evaporation rate	Not applicable
Flammability	No information available
Upper/lower explosive limits[%(v/v)]	Upper limit : 4.5 ; Lower limit : 0.7
Vapor pressure	0.04Pa (20°C)
Vapor density(Air = 1)	> 1
Relative density(Water=1)	1.06
Solubility	15mg/L (23 °C)
n-octanol/water partition coefficient	4.75 (calculated)
Auto-ignition temperature(°C)	430
Decomposition temperature(°C)	310
Kinematic viscosity	Not applicable
Explosive properties	No information available
Oxidizing properties	No information available
Particle characteristics	No information available

9.2 Other information

9.2.1 Information with regard to physical hazard classes

Information with regard to physical hazard classes	No information available
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9.2.2 Other safety characteristics

Other safety characteristics	No information available
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10 Stability and reactivity

Stability and reactivity

10.1 Reactivity	Contact with incompatible substances can cause decomposition or other chemical reactions.
10.2 Chemical stability	Stable under proper operation and storage conditions.
10.3 Possibility of hazardous reactions	No information available.
10.4 Conditions to avoid	Incompatible materials, heat, flame and spark.
10.5 Incompatible materials	No information available.
10.6 Hazardous decomposition products	Under normal conditions of storage and use, hazardous decomposition products should not be produced.

11 Toxicological information

11.1 Information on hazard classes as defined in Regulation (EC) No 1272/2008 with amendment 2023/707

3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate(Component)	
Skin corrosion/irritation	Causes skin irritation(Category 2)
Serious eye damage/irritation	Causes serious eye irritation(Category 2)
Skin sensitization	May cause an allergic skin reaction(Category 1)
Respiratory sensitization	May cause allergy or asthma symptoms or breathing difficulties if inhaled(Category 1)
Reproductive toxicity	Based on available data, the classification criteria are not met
STOT-single exposure	May cause respiratory irritation(Category 3)
STOT-repeated exposure	Based on available data, the classification criteria are not met
Aspiration hazard	Based on available data, the classification criteria are not met
Germ cell mutagenicity	Based on available data, the classification criteria are not met

Acute toxicity

Component	LD ₅₀ (oral)	LD ₅₀ (dermal)	LC ₅₀ (inhalation,4h)
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	4825mg/kg(Rat)	No information available	0.031mg/L(Rat)

Carcinogenicity

Component	List of carcinogens by the IARC Monographs	Report on Carcinogens by NTP
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	Not Listed	Not Listed

11.2 Information on other hazards

11.2.1 Endocrine disrupting properties

Component	Endocrine disrupting properties
3-isocyanatomethyl-3,5,5-t	No information available

rimethylcyclohexyl isocyanate	
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11.2.2 Other Information

Other Information	See Section 11.1
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12 Ecological information

12.1 Toxicity

Acute aquatic toxicity

Acute aquatic toxicity	No information available
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Chronic aquatic toxicity

Chronic aquatic toxicity	No information available
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12.2 Persistence and degradability

Persistence and degradability	No information available
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12.3 Bioaccumulative potential

Bioaccumulative potential	No information available
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12.4 Mobility in soil

Component	log Koc	Remark
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	4.562	

12.5 Results of PBT and vPvB assessment

Component	Results of PBT and vPvB assessment [according to (EC) No 1907/2006]
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	Not PBT/vPvB

12.6 Endocrine disrupting properties

Component	Endocrine disrupting properties
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	No information available

12.7 Other adverse effects

	No information available
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13 Disposal considerations

13.1 Waste treatment methods

Waste chemicals	Before disposal should refer to the relevant national and local laws and regulation. Recommend the use of incineration disposal.
Contaminated packaging	Containers may still present chemical hazard when empty. Keep away from hot and ignition source of fire. Return to supplier for recycling if possible.

Disposal recommendations

Refer to section waste chemicals and contaminated packaging.

14 Transport information**| Label and Mark**

Transporting Label	
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| IMDG-CODE

14.1 UN number	2290
14.2 UN proper shipping name	ISOPHORONE DIISOCYANATE
14.3 Transport hazard class	6.1
14.4 Packing group	III
14.5 Environmental hazards (Yes or no)	Yes

| IATA-DGR

14.1 UN number	2290
14.2 UN proper shipping name	ISOPHORONE DII SOCYANATE
14.3 Transport hazard class	6.1
14.4 Packing group	III
14.5 Environmental hazards (Yes or no)	Yes

| UN-ADR

14.1 UN number	2290
14.2 UN proper shipping name	ISOPHORONE DIISOCYANATE
14.3 Transport hazard class	6.1
14.4 Packing group	III
14.5 Environmental hazards (Yes or no)	Yes

| Special precautions for user

	Transit should be anti-exposure, rain, high temperature. Strictly prohibited shipping or transportation with acids, alkalis, oxidants, food and food additives etc. Transport vehicles should be equipped with the appropriate variety and quantity of fire equipment and emergency equipment leakage during transport. Before transport, should be preceded by checking whether container integrity, sealing. The transport unit must be placarded and marked in accordance with relevant transporting requirements.
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| Maritime transport in bulk according to IMO instruments

- ◆ Transport in bulk according to Annex II of MARPOL and the IBC code

	Not Available
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- ◆ Transport in bulk in accordance with MARPOL Annex V and the IMSBC Code

	Not Available
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- ◆ Transport in bulk in accordance with the IGC Code

Not Available

15 Regulatory information

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

International chemical inventory

Component	A	B	C	D	E	F	G	H	I	J	K	L	M
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

- [A] China Inventory of Existing Chemical Substances(IECSC)
 [B] European Inventory of Existing Commercial Chemical Substances(EC inventory)
 [C] United States Toxic Substances Control Act Inventory(TSCA)
 [D] Canadian Domestic Substances List(DSL)
 [E] New Zealand Inventory of Chemicals(NZIoC)
 [F] Philippines Inventory of Chemicals and Chemical Substances(PICCS)
 [G] Korea Existing Chemicals Inventory(KECL)
 [H] Australian. Inventory of Industrial Chemical (AIICS)
 [I] Japan Inventory of Existing & New Chemical Substances(ENCS)
 [J] Thailand Existing Chemicals Inventory(TECI)
 [K] Mexico National Inventory of Chemical Substances (INSQ)
 [L] Russia Inventory of Existing Substances(DRAFT)
 [M] Inventory of Existing Chemical Substances in Taiwan, China (TCSI)

List of Chemical Substances under International Conventions

Component	A	B	C
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	×	×	×

- [A] The Montreal Protocol on Substances that Deplete the Ozone Layer
 [B] Stockholm Convention on Persistent Organic Pollutants (POPs)
 [C] Rotterdam Convention on the prior informed consent procedure for certain hazardous chemicals and pesticides in international trade

European chemical inventory

Component	A	B	C	D	E	F	G	H	I
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	×	×	✓	✓	✓	×	×	×	×

- [A] Candidate list of Substances of Very High Concern for authorization under EU REACH regulation
 [B] Substances requiring authorisation under EU REACH regulation
 [C] Substances restricted under EU REACH
 [D] Pre-registered substances under EU REACH
 [E] Registered substances under EU REACH
 [F] Substance Evaluation – CoRAP under EU REACH
 [G] List of priority substances under EU water policy (Directive 2455/2001/EC)
 [H] Substances subject to POPs Regulation
 [I] Substances proposed as POPs

Note:

“✓” Indicates that the substance included in the regulations.

“×” No data or not included in the regulations.

German water hazard class(WGK)

Component	WGK	Remark
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	WGK 2	

【WGK 1】 slightly hazardous to water
 【WGK 2】 obviously hazardous to water
 【WGK 3】 highly hazardous to water
 【nwg】 non-hazardous to water
 【awg】 hazardous to water in general

German technical instructions on air quality control(TA LUFT)

Component	TA LUFT	Remark
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	Chapter 5.2.5 Organic Substances, class I. The following values are in all not allowed to be exceeded in the exhaust gas: Mass flow: 0,10 kg/hr or Mass conc.: 20 mg/m ³	

German technical rules for hazardous substances(TRGS)

Component	TRGS	Remark
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	TRGS 201 TRGS 400 TRGS 555 TRGS 600 TRGS 402 TRGS 401 TRGS 406 TRGS 500 TRGS 509 TRGS 510 TRGS 800 TRGS 430	

15.2 Chemical safety assessment

	No Chemical Safety Assessment has been carried out for this substance/mixture by the supplier.
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16 Other information

Information on revision

Creation Date	2026/01/16
Revision Date	-
Reason for revision	-

Reference

- [1] IPCS: The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>.
- [2] IARC, website: <http://www.iarc.fr/>.
- [3] OECD: The Global Portal to Information on Chemical Substances, website: <https://www.echemportal.org/echemportal/>.
- [4] CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>.
- [5] NLM: ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>.
- [6] EPA: Integrated Risk Information System, website: <http://cfpub.epa.gov/iris/>.
- [7] U.S. Department of Transportation: ERG, website: <http://www.phmsa.dot.gov/hazmat/library/erg>.
- [8] Germany GESTIS-database on hazard substance, website: <http://gestis-en.itrust.de/>.

Abbreviations and acronyms

CAS	Chemical Abstracts Service	UN	The United Nations
PC-STEL	Short term exposure limit	OECD	Organization for Economic Co-operation and Development
PC-TWA	Time Weighted Average	IMDG-CODE	International Maritime Dangerous Goods CODE
MAC	Maximum Allowable Concentration	IARC	International Agency for Research on Cancer
DNEL	Derived No Effect Level	ICAO	International Civil Aviation Organization
PNEC	Predicted No Effect Concentration	IATA	International Air Transportation Association
NOEC	No Observed Effect Concentration	ACGIH	American Conference of Governmental Industrial Hygienists

LC ₅₀	Lethal Concentration 50%	NFPA	National Fire Protection Association
LD ₅₀	Lethal Dose 50%	NTP	National Toxicology Program
EC ₅₀	Effective Concentration 50%	PBT	Persistent, Bioaccumulative, Toxic
EC _x	Effective Concentration X%	vPvB	very Persistent, very Bioaccumulative
P _{ow}	Partition coefficient Octanol: Water	CMR	Carcinogens, mutagens or substances toxic to reproduction
BCF	Bioconcentration factor	RPE	Respiratory Protective Equipment
ED	Endocrine disruptor		

Disclaimer

This Safety Data Sheet (SDS) was prepared according to REACH Regulation. The data included was derived from international authoritative database and provided by the enterprise. Other information was based on the present state of our knowledge. We try to ensure the correctness of all information. However, due to the diversity of information sources and the limitations of our knowledge, this document is only for user's reference. Users should make their independent judgment of suitability of this information for their particular purposes. We do not assume responsibility for loss, damage or expense arising out of or in any way connected with the handling, storage, use or disposal of the product.