

according to Regulation UK SI 2019/758 and UK SI 2020/1577 as amended

Creation Date 22-Jun-2009

Revision Date 20-Feb-2024

Revision Number 13

## SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

## 1.1. Product identifier

Product Description:	2,2,4-Trimethylpentane
Cat No. :	421980000; 421980025; 421980040; 421985000
Synonyms	Isooctane
Index No	601-009-00-8
CAS No	540-84-1
EC No	208-759-1
Molecular Formula	C8 H18

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

Recommended Use Sector of use	Laboratory chemicals. SU3 - Industrial uses: Uses of substances as such or in preparations at industrial sites
Product category	PC21 - Laboratory chemicals
Process categories	PROC15 - Use as a laboratory reagent
Environmental release category	ERC6a - Industrial use resulting in manufacture of another substance (use of intermediates)
Uses advised against	No Information available

## 1.3. Details of the supplier of the safety data sheet

Company	<b>UK entity/business name</b> Fisher Scientific UK Bishop Meadow Road, Loughborough, Leicestershire LE11 5RG, United Kingdom <b>EU entity/business name</b> Thermo Fisher Scientific Janssen Pharmaceuticalaan 3a, 2440 Geel, Belgium
E-mail address	begel.sdsdesk@thermofisher.com
1.4. Emergency telephone number	For information <b>US</b> call: 001-800-227-6701 / <b>Europe</b> call: +32 14 57 52 11 Emergency Number <b>US:</b> 001-201-796-7100 / <b>Europe:</b> +32 14 57 52 99 <b>CHEMTREC</b> Tel. No. <b>US:</b> 001-800-424-9300 / <b>Europe:</b> 001-703-527-3887

## **SECTION 2: HAZARDS IDENTIFICATION**

## 2.1. Classification of the substance or mixture

CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567

## **Physical hazards**

## 2,2,4-Trimethylpentane

#### Revision Date 20-Feb-2024

Category 1 (H410)

Flammable liquids	Category 2 (H225)
Health hazards	
Aspiration Toxicity Skin Corrosion/Irritation Specific target organ toxicity - (single exposure)	Category 1 (H304) Category 2 (H315) Category 3 (H336)
Environmental hazards	
Acute aquatic toxicity	Category 1 (H400)

Full text of Hazard Statements: see section 16

Chronic aquatic toxicity



Signal Word

Danger

#### **Hazard Statements**

- H225 Highly flammable liquid and vapor
- H304 May be fatal if swallowed and enters airways
- H315 Causes skin irritation
- H336 May cause drowsiness or dizziness
- H410 Very toxic to aquatic life with long lasting effects

## **Precautionary Statements**

- P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician
- P331 Do NOT induce vomiting
- P280 Wear protective gloves/protective clothing
- P304 + P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing
- P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower
- P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking

## 2.3. Other hazards

Substance is not considered persistent, bioaccumulative and toxic (PBT) / very persistent and very bioaccumulative (vPvB)

This product does not contain any known or suspected endocrine disruptors

## **SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS**

## 3.1. Substances

Component	CAS No	EC No	Weight %	CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
Isooctane	540-84-1	EEC No. 208-759-1	>95	Flam. Liq. 2 (H225)

## 2,2,4-Trimethylpentane

#### Revision Date 20-Feb-2024

	Asp. Tox. 1 (H304) Skin Irrit. 2 (H315) STOT SE 3 (H336) Aquatic Acute 1 (H400) Aquatic Chronic 1 (H410)
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Component	Specific concentration limits (SCL's)	M-Factor	Component notes
Isooctane	-	1	-

#### Full text of Hazard Statements: see section 16

## **SECTION 4: FIRST AID MEASURES**

#### 4.1. Description of first aid measures

General Advice	If symptoms persist, call a physician.
General Advice	
Eye Contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.
Ingestion	Clean mouth with water and drink afterwards plenty of water. Do NOT induce vomiting. Call a physician or poison control center immediately. If vomiting occurs naturally, have victim lean forward.
Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur. Risk of serious damage to the lungs (by aspiration).
Self-Protection of the First Aider	Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.
4.2. Most important symptoms and	effects, both acute and delayed
	None reasonably foreseeable. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting
4.3. Indication of any immediate me	dical attention and special treatment needed

Notes to Physician Trea	t symptomatically. Symptoms may be delayed.
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## **SECTION 5: FIREFIGHTING MEASURES**

## 5.1. Extinguishing media

## Suitable Extinguishing Media

Water spray, carbon dioxide (CO2), dry chemical, alcohol-resistant foam. Water mist may be used to cool closed containers.

#### **Extinguishing media which must not be used for safety reasons** Do not use a solid water stream as it may scatter and spread fire.

Do not use a solid water stream as it may scatter and spread life.

## 5.2. Special hazards arising from the substance or mixture

Flammable. Risk of ignition. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Containers may explode when heated. Vapors may form explosive mixtures with air. Do not allow run-off from fire-fighting to enter drains or water courses.

#### **Hazardous Combustion Products**

## 2,2,4-Trimethylpentane

Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>).

#### 5.3. Advice for firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

## **SECTION 6: ACCIDENTAL RELEASE MEASURES**

#### 6.1. Personal precautions, protective equipment and emergency procedures

Use personal protective equipment as required. Ensure adequate ventilation. Remove all sources of ignition. Take precautionary measures against static discharges.

## 6.2. Environmental precautions

Do not flush into surface water or sanitary sewer system. Do not allow material to contaminate ground water system. Prevent product from entering drains. Local authorities should be advised if significant spillages cannot be contained.

## 6.3. Methods and material for containment and cleaning up

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

#### 6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

## **SECTION 7: HANDLING AND STORAGE**

## 7.1. Precautions for safe handling

Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. To avoid ignition of vapors by static electricity discharge, all metal parts of the equipment must be grounded. Take precautionary measures against static discharges.

#### **Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

#### 7.2. Conditions for safe storage, including any incompatibilities

Keep away from open flames, hot surfaces and sources of ignition. Keep containers tightly closed in a dry, cool and well-ventilated place. Flammables area. Keep away from heat, sparks and flame.

Technical Rules for Hazardous Substances (TRGS) 510 Class 3 Storage Class (LGK) (Germany)

## 7.3. Specific end use(s)

Use in laboratories

## **SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION**

## **Exposure limits**

List source(s):

## **Biological limit values**

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

## Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

See table for values

Component	Acute effects local	Acute effects	Chronic effects local	Chronic effects
	(Oral)	systemic (Oral)	(Oral)	systemic (Oral)
Isooctane 540-84-1(>95)				699 mg/kg bw/day

Component	Acute effects local (Dermal)	Acute effects systemic (Dermal)	Chronic effects local (Dermal)	Chronic effects systemic (Dermal)
Isooctane 540-84-1(>95)				DNEL = 773mg/kg bw/day

Component	Acute effects local (Inhalation)	Acute effects systemic (Inhalation)	Chronic effects local (Inhalation)	Chronic effects systemic (Inhalation)
Isooctane 540-84-1(>95)				DNEL = 2035mg/m <sup>3</sup>

## Predicted No Effect Concentration (PNEC)

No information available.

## 8.2. Exposure controls

## **Engineering Measures**

Use only under a chemical fume hood. Use explosion-proof electrical/ventilating/lighting equipment. Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

## Personal protective equipment

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Eye Protection
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Wear safety glasses with side shields (or goggles) (European standard - EN 166)

Hand	Protection
nanu	FIOLECTION

Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	> 480 minutes	0.3 mm	Level 6	As tested under EN374-3 Determination of
Viton (R) Neoprene	> 480 minutes	0.35 mm	EN 374	Resistance to Permeation by Chemicals
Natural rubber				
PVC				
Neoprene gloves	> 480 minutes	0.45 mm		

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatability, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Respiratory Protection	When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.
Large scale/emergency use	Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced <b>Recommended Filter type:</b> Organic gases and vapours filter Type A Brown conforming to EN371
Small scale/Laboratory use	Maintain adequate ventilation Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced. <b>Recommended half mask:-</b> Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 371
Environmental exposure controls	Prevent product from entering drains. Do not allow material to contaminate ground water

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Environmental exposure controls Prevent product from entering drains. Do not allow material to contaminate ground wate system. Local authorities should be advised if significant spillages cannot be contained.
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## **SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES**

## 9.1. Information on basic physical and chemical properties

Physical State	Liquid	
Appearance Odor Odor Threshold Melting Point/Range Softening Point	Colorless Petroleum distillates No data available -107 °C / -160.6 °F No data available	
Boiling Point/Range	98 - 99 °C / 208.4 - 210.2 °F	@ 760 mmHg
Flammability (liquid) Flammability (solid,gas)	Highly flammable Not applicable	On basis of test data Liguid
Explosion Limits	Lower 1.1 vol %	Elquid
	Upper 6 vol %	
Flash Point	-12 °C / 10.4 °F	Method - No information available
Autoignition Temperature	410 °C / 770 °F	
Decomposition Temperature	No data available	
pH Viecesity	Not applicable	
Viscosity Water Solubility	0.51 mPa s at 22 °C Immiscible	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/wate		
Vapor Pressure	51 mbar @ 20 °C	
Density / Specific Gravity	0.690	
Bulk Density	Not applicable	Liquid
Vapor Density	3.94	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	
9.2. Other information		
Molecular Formula	C8 H18	
Molecular Weight	114.23	

# **Explosive Properties** Vapors may form explosive mixtures with air

## **SECTION 10: STABILITY AND REACTIVITY**

10.2. Chemical stability	Stable under normal conditions.
10.3. Possibility of hazardous react	ions
Hazardous Polymerization Hazardous Reactions	Hazardous polymerization does not occur. None under normal processing.
10.4. Conditions to avoid	Incompatible products. Heat, flames and sparks. Keep away from open flames, hot surfaces and sources of ignition.
10.5. Incompatible materials	Strong oxidizing agents. Strong acids. Strong bases.

## 10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

## **SECTION 11: TOXICOLOGICAL INFORMATION**

## 11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

## **Product Information**

(a) acute toxicity;

OralBased on available data, the classification criteria are not metDermalBased on available data, the classification criteria are not metInhalationBased on available data, the classification criteria are not met

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Isooctane	LD50 5000 mg/kg (Rat)	2000 mg/kg (Rabbit)	LC50 = 33.52 mg/L (Rat) 4 h

(b) skin corrosion/irritation;	Category 2
(c) serious eye damage/irritation;	Based on available data, the classification criteria are not met
(d) respiratory or skin sensitization Respiratory Skin	; Based on available data, the classification criteria are not met Based on available data, the classification criteria are not met
(e) germ cell mutagenicity;	Based on available data, the classification criteria are not met
(f) carcinogenicity;	Based on available data, the classification criteria are not met
	There are no known carcinogenic chemicals in this product
(g) reproductive toxicity;	Based on available data, the classification criteria are not met
(h) STOT-single exposure;	Category 3
Effective dose Results / Target organs	NOAEL 2220 ppm 6hr/day Central nervous system (CNS).
(i) STOT-repeated exposure;	Based on available data, the classification criteria are not met

## 2,2,4-Trimethylpentane

Target Organs	None known.
(j) aspiration hazard;	Category 1
Other Adverse Effects	The toxicological properties have not been fully investigated.
Symptoms / effects,both acute and delayed	Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting.

## 11.2. Information on other hazards

 Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

# SECTION 12: ECOLOGICAL INFORMATION

## 12.1. Toxicity Ecotoxicity effects

Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment. The product contains following substances which are hazardous for the environment.

Component	Freshwater Fish	Water Flea	Freshwater Algae
Isooctane	LC50 = 0.11 mg/l, 96h, (Rainbow	EC50= 0.4 mg/l, 48h (Daphnia	EC50= 2.94 mg/l, 72h
	trout)	magna)	

Component	Microtox	M-Factor
Isooctane		1

## 12.2. Persistence and degradability

12.2. Persistence and degradability	
Persistence	Insoluble in water, Persistence is unlikely, based on information available, Immiscible with
	water.
Degradation in sewage	Contains substances known to be hazardous to the environment or not degradable in waste
treatment plant	water treatment plants.
F	
12.3. Bioaccumulative potential	May have some potential to bioaccumulate
Bioconcentration factor (BCF)	231
<u>12.4. Mobility in soil</u>	Spillage unlikely to penetrate soil The product is insoluble and floats on water The product
	contains volatile organic compounds (VOC) which will evaporate easily from all surfaces
	Will likely be mobile in the environment due to its volatility. Is not likely mobile in the
	environment due its low water solubility.
12.5. Results of PBT and vPvB	Substance is not considered persistent, biogeourgulative and taxis (DBT) / yes/ persistent
	Substance is not considered persistent, bioaccumulative and toxic (PBT) / very persistent
assessment	and very bioaccumulative (vPvB).
40.C. Endeering discusting	
12.6. Endocrine disrupting	
properties	This product door not contain only because of our production discussion.
Endocrine Disruptor Information	This product does not contain any known or suspected endocrine disruptors
12.7. Other adverse effects	
Persistent Organic Pollutant	This product does not contain any known or suspected substance
Ozone Depletion Potential	This product does not contain any known or suspected substance
-	

## **SECTION 13: DISPOSAL CONSIDERATIONS**

#### 13.1. Waste treatment methods Waste from Residues/Unused Waste is classified as hazardous. Dispose of in accordance with the European Directives Products on waste and hazardous waste. Dispose of in accordance with local regulations. **Contaminated Packaging** Dispose of this container to hazardous or special waste collection point. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and empty container away from heat and sources of ignition. European Waste Catalogue (EWC) According to the European Waste Catalog, Waste Codes are not product specific, but application specific. Do not flush to sewer. Waste codes should be assigned by the user based on the **Other Information** application for which the product was used. Can be landfilled or incinerated, when in compliance with local regulations. Do not let this chemical enter the environment. Do not empty into drains.

## **SECTION 14: TRANSPORT INFORMATION**

## IMDG/IMO

14.1. UN number	UN1262
14.2. UN proper shipping name	OCTANES
14.3. Transport hazard class(es)	3
14.4. Packing group	II

ADR

<u>14.1. UN number</u>	UN1262
14.2. UN proper shipping name	OCTANES
14.3. Transport hazard class(es)	3
14.4. Packing group	Π

IATA

<u>14.1. UN number</u> <u>14.2. UN proper shipping name</u> <u>14.3. Transport hazard class(es)</u> <u>14.4. Packing group</u>	UN1262 OCTANES 3 II
14.5. Environmental hazards	Dangerous for the environment Product is a marine pollutant according to the criteria set by IMDG/IMO
14.6. Special precautions for user	No special precautions required.
14.7. Maritime transport in bulk according to IMO instruments	Not applicable, packaged goods

## **SECTION 15: REGULATORY INFORMATION**

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

#### International Inventories

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

## 2,2,4-Trimethylpentane

Isooctane

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Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
Isooctane	540-84-1	208-759-1	-	-	Х	Х	KE-34634	Х	Х
Component	CAS No	TSCA	TSCA Ir	ventory	DSL	NDSL	AICS	NZIoC	PICCS
			notific	ation -					1

ACTIVE

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Х Legend: X - Listed '-' - Not Listed KECL - NIER number or KE number (http://ncis.nier.go.kr/en/main.do)

540-84-1

#### Authorisation/Restrictions according to EU REACH

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	5	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Isooctane	540-84-1	-	Use restricted. See item 75. (see link for restriction details)	-

#### **REACH links**

https://echa.europa.eu/substances-restricted-under-reach

## Seveso III Directive (2012/18/EC)

Component	CAS No	Seveso III Directive (2012/18/EC) - Seveso III Directive (2012/	
-		Qualifying Quantities for Major Accident Qualifying Quantities for Safety I	
		Notification	Requirements
Isooctane	540-84-1	Not applicable	Not applicable

## Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

## Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)? Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

## **National Regulations**

UK - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

## WGK Classification

See table for values

Component	Germany - Water Classification (AwSV)	Germany - TA-Luft Class
Isooctane	WGK2	

Component	Switzerland - Ordinance on the Reduction of Risk from handling of hazardous substances preparation (SR 814.81)	Switzerland - Ordinance of the Rotterdam Convention on the Prior Informed Consent Procedure
Isooctane	Prohibited and Restricted	

2,2,4-Trimethylpentane

Revision Date 20-Feb-2024

540-84-1 (>95)

Substances

## 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

## **SECTION 16: OTHER INFORMATION**

## Full text of H-Statements referred to under sections 2 and 3

H304 - May be fatal if swallowed and enters airways

H315 - Causes skin irritation

H336 - May cause drowsiness or dizziness

- H400 Very toxic to aquatic life
- H410 Very toxic to aquatic life with long lasting effects
- H225 Highly flammable liquid and vapor

## Legend

CAS - Chemical Abstracts Service	<b>TSCA</b> - United States Toxic Substances Control Act Section 8(b) Inventory
<b>EINECS/ELINCS</b> - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances <b>PICCS</b> - Philippines Inventory of Chemicals and Chemical Substances <b>IECSC</b> - Chinese Inventory of Existing Chemical Substances <b>KECL</b> - Korean Existing and Evaluated Chemical Substances	,

WEL - Workplace Exposure Limit ACGIH - American Conference of Governmental Industrial Hygienists DNEL - Derived No Effect Level RPE - Respiratory Protective Equipment LC50 - Lethal Concentration 50% NOEC - No Observed Effect Concentration PBT - Persistent, Bioaccumulative, Toxic

ADR - European Agreement Concerning the International Carriage of<br/>Dangerous Goods by RoadICAO/<br/>TranspIMO/IMDG - International Maritime Organization/International Maritime<br/>Dangerous Goods CodeMARP<br/>ShipsOECD - Organisation for Economic Co-operation and Development<br/>BCF - Bioconcentration factorATE -<br/>VOC -<br/>VOC -Key literature references and sources for data<br/>https://echa.europa.eu/information-on-chemicals<br/>Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

 IARC - International Agency for Research on Cancer Predicted No Effect Concentration (PNEC)
LD50 - Lethal Dose 50%
EC50 - Effective Concentration 50%
POW - Partition coefficient Octanol:Water vPvB - very Persistent, very Bioaccumulative
ICAO/IATA - International Civil Aviation Organization/International Air Transport Association
MARPOL - International Convention for the Prevention of Pollution from

MARPOL - International Convention for the Prevention of Pollution from Ships ATE - Acute Toxicity Estimate

VOC - (Volatile Organic Compound)

TWA - Time Weighted Average

## Training Advice

Chemical incident response training.

Creation Date	22-Jun-2009
Revision Date	20-Feb-2024
Revision Summary	Not applicable.

# This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.

## Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

# End of Safety Data Sheet