

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

Revision Date 30-Jan-2024 Revision Number 3

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

#### 1.1. Product identifier

Product Description: 2,6-Dimethyl-4-heptanone, (sum of 2,6-Dimethyl-4-heptanone &

4,6-Dimethyl-2-heptanone)

Cat No. : L16015

**Synonyms** 2,6-Dimethyl-4-heptanone.; Isobutyl Ketone

 Index No
 606-005-00-X

 CAS No
 108-83-8

 Molecular Formula
 C9 H18 O

REACH registration number -

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

Recommended Use Laboratory chemicals.

Sector of use 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

Avocado Research Chemicals Ltd. (Part of Thermo Fisher Scientific)

Shore Road, Heysham Lancashire, LA3 2XY, United Kingdom

Office Tel: +44 (0) 1524 850506 Office Fax: +44 (0) 1524 850608

E-mail address begel.sdsdesk@thermofisher.com

1.4. Emergency telephone number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11 Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99 **CHEMTREC** Tel. No. **US**:001-800-424-9300 / **Europe**: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** 

ALFAAL16015

2,6-Dimethyl-4-heptanone, (sum of 2,6-Dimethyl-4-heptanone & 4,6-Dimethyl-2-heptanone)

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Flammable liquids Category 3 (H226)

**Health hazards** 

Specific target organ toxicity - (single exposure)

Category 3 (H335)

**Environmental hazards** 

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

#### 2.2. Label elements



#### Signal Word

#### Warning

#### **Hazard Statements**

H226 - Flammable liquid and vapor

H335 - May cause respiratory irritation

#### **Precautionary Statements**

P261 - Avoid breathing dust/fume/gas/mist/vapors/spray

P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing

P312 - Call a POISON CENTER or doctor if you feel unwell

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed

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)

Toxicity to Soil Dwelling Organisms

Toxic to terrestrial vertebrates

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
Diisobutylketone	108-83-8	EEC No. 203-620-1	100	Flam. Liq. 3 (H226) STOT SE 3 (H335)

Component Specific concentration limits	M-Factor	Component notes
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	(SCL's)		
Diisobutylketone	STOT SE 3 (H335) :: C>=10%	-	-

REACH registration number	-

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.

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.

**Inhalation** Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if

symptoms occur.

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

Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness,

nausea and vomiting

4.3. Indication of any immediate medical attention and special treatment needed

**Notes to Physician** Treat symptomatically. Symptoms may be delayed.

#### **SECTION 5: FIREFIGHTING MEASURES**

## 5.1. Extinguishing media

#### **Suitable Extinguishing Media**

Water spray. Carbon dioxide (CO<sub>2</sub>). Dry chemical. Chemical foam. Water mist may be used to cool closed containers.

#### Extinguishing media which must not be used for safety reasons

No information available.

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

Flammable. Vapors may form explosive mixtures with air. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Combustible material.

#### **Hazardous Combustion Products**

Carbon monoxide (CO), Carbon dioxide (CO2).

#### 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.

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

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

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

#### 6.2. Environmental precautions

Should not be released into the environment. See Section 12 for additional Ecological Information.

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

Keep in suitable, closed containers for disposal. Soak up with inert absorbent material. 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. 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 in a dry, cool and well-ventilated place. Keep container tightly closed. Keep away from heat, sparks and flame. Flammables area. Keep containers tightly closed in a dry, cool and well-ventilated place.

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**

#### 8.1. Control parameters

## **Exposure limits**

List source(s): **UK** - EH40/2005 Work Exposure Limits, Fourth edition. Published 2020. **IRE** - 2021 Code of Practice for the Chemical Agents Regulations, Schedule 1. Published by the Health and Safety Authority

Component	The United Kingdom	European Union	Ireland
Diisobutylketone	STEL: 75 ppm 15 min		TWA: 25 ppm 8 hr.
·	STEL: 444 mg/m <sup>3</sup> 15 min		TWA: 150 mg/m <sup>3</sup> 8 hr.

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TIA(A 05 01	OTEL 75 45 :
TWA: 25 ppm 8 hr	STEL: 75 ppm 15 min
TWA: 148 mg/m <sup>3</sup> 8 hr	STEL: 450 mg/m <sup>3</sup> 15 min

#### **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 (Dermal)	Acute effects systemic (Dermal)	Chronic effects local (Dermal)	Chronic effects systemic (Dermal)
Diisobutylketone 108-83-8 ( 100 )				DNEL = 7.7mg/kg bw/day

Component	Acute effects local (Inhalation)	Acute effects systemic (Inhalation)	Chronic effects local (Inhalation)	Chronic effects systemic (Inhalation)
Diisobutylketone 108-83-8 ( 100 )				DNEL = 53mg/m <sup>3</sup>

#### **Predicted No Effect Concentration (PNEC)**

See values below.

	Component	Fresh water	Fresh water	Water Intermittent	Microorganisms in	Soil (Agriculture)
			sediment		sewage treatment	
Γ	Diisobutylketone	PNEC = 0.03mg/L	PNEC = 0.46mg/kg	PNEC = 0.3mg/L	PNEC = 2.55mg/L	PNEC =
	108-83-8 ( 100 )		sediment dw			0.0746mg/kg soil
						dw

Component	Marine water	Marine water sediment	Marine water intermittent	Food chain	Air
Diisobutylketone	PNEC = 0.003mg/L	PNEC =			
108-83-8 ( 100 )		0.046mg/kg			
		sediment dw			

#### 8.2. Exposure controls

#### **Engineering Measures**

Ensure adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting equipment. Ensure that eyewash stations and safety showers are close to the workstation location.

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

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

Hand Protection Protective gloves

	Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
١	Viton (R)	See manufacturers	-	EN 374	(minimum requirement)
		recommendations			

**Skin and body protection** Long sleeved clothing.

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

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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.

To protect the wearer, respiratory protective equipment must be the correct fit and be used

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and maintained properly

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

Recommended Filter type: Organic gases and vapours filter Type A Brown conforming to

EN14387

Small scale/Laboratory use 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.

Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN

When RPE is used a face piece Fit Test should be conducted

**Environmental exposure controls** No information available.

#### **SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES**

#### 9.1. Information on basic physical and chemical properties

**Physical State** Liquid

**Appearance** Light yellow Odor Mint-like

**Odor Threshold** No data available **Melting Point/Range** -46 °C / -50.8 °F **Softening Point** No data available

**Boiling Point/Range** 166 °C / 330.8 °F @ 760 mmHg Flammability (liquid) Flammable On basis of test data Liquid

Flammability (solid,gas) Not applicable No data available

**Explosion Limits** 

60 °C / 140 °F **Flash Point** Method - No information available

345 °C / 653 °F **Autoignition Temperature** No data available **Decomposition Temperature** pН No information available **Viscosity** 1.05 mPa s at 20 °C

**Water Solubility** No information available Solubility in other solvents No information available

Partition Coefficient (n-octanol/water)

Component log Pow Diisobutylketone 3.71

1 hPa @ 20 °C **Vapor Pressure** 

**Density / Specific Gravity** 0.809

**Bulk Density** Not applicable Liquid **Vapor Density** 4.9 (Air = 1.0)

Particle characteristics Not applicable (liquid)

#### 9.2. Other information

C9 H18 O Molecular Formula **Molecular Weight** 142.24

**Explosive Properties** explosive air/vapour mixtures possible

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

2,6-Dimethyl-4-heptanone, (sum of 2,6-Dimethyl-4-heptanone & 4,6-Dimethyl-2-heptanone)

10.1. Reactivity None known, based on information available

10.2. Chemical stability

Stable.

10.3. Possibility of hazardous reactions

**Hazardous Polymerization** Hazardous polymerization does not occur.

**Hazardous Reactions** None under normal processing.

10.4. Conditions to avoid

Keep away from open flames, hot surfaces and sources of ignition. Incompatible products.

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10.5. Incompatible materials

Strong oxidizing agents. Strong bases. Strong reducing agents.

10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO2).

## **SECTION 11: TOXICOLOGICAL INFORMATION**

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

#### **Product Information**

(a) acute toxicity;

Based on available data, the classification criteria are not met Oral **Dermal** Based on available data, the classification criteria are not met Inhalation Based on available data, the classification criteria are not met

Component	ponent LD50 Oral		LC50 Inhalation	
Diisobutylketone	LD50 = 5750 mg/kg (Rat)	LD50 > 2000 mg/kg (Rat)	LC50 > 2300 ppm (Rat) 4 h	

Based on available data, the classification criteria are not met (b) skin corrosion/irritation;

Based on available data, the classification criteria are not met (c) serious eye damage/irritation;

(d) respiratory or skin sensitization;

Respiratory Based on available data, the classification criteria are not met Skin

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

Category 3 (h) STOT-single exposure;

Results / Target organs Respiratory system.

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(i) STOT-repeated exposure; Based on available data, the classification criteria are not met

Target Organs None known.

(j) aspiration hazard; Based on available data, the classification criteria are not met

Symptoms / effects, both acute and Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting.

delayed

11.2. Information on other hazards

Endocrine Disrupting Properties 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**Do not flush into surface water or sanitary sewer system. Do not allow material to

contaminate ground water system. Do not empty into drains.

Component	Freshwater Fish	Water Flea	Freshwater Algae
Diisobutylketone	LC50: 140 mg/L, 96h semi-static (Oncorhynchus mykiss)		EC50: 100 mg/L, 96h (Pseudokirchneriella subcapitata)

#### 12.2. Persistence and degradability No information available

## **12.3. Bioaccumulative potential** No information available

Component	log Pow	Bioconcentration factor (BCF)
Diisobutylketone	3.71	No data available

**12.4. Mobility in soil** No information available

12.5. Results of PBT and vPvB Substance is not considered persistent, bioaccumulative and toxic (PBT) / very persistent

<u>assessment</u> and very bioaccumulative (vPvB).

12.6. Endocrine disrupting

properties

Endocrine Disruptor Information This product does not contain any known or suspected endocrine disruptors

12.7. Other adverse effects

Persistent Organic Pollutant
Ozone Depletion Potential

This product does not contain any known or suspected substance
This product does not contain any known or suspected substance

## **SECTION 13: DISPOSAL CONSIDERATIONS**

## 13.1. Waste treatment methods

Waste from Residues/Unused Products

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

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**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.

Other Information Waste codes should be assigned by the user based on the application for which the product

was used. Do not flush to sewer. Can be landfilled or incinerated, when in compliance with

local regulations.

## **SECTION 14: TRANSPORT INFORMATION**

#### IMDG/IMO

**14.1. UN number** UN1157

14.2. UN proper shipping name DIISOBUTYL KETONE

14.3. Transport hazard class(es) 3 14.4. Packing group III

#### ADR

**14.1. UN number** UN1157

14.2. UN proper shipping name DIISOBUTYL KETONE

14.3. Transport hazard class(es) 3 14.4. Packing group III

## <u>IATA</u>

**14.1. UN number** UN1157

14.2. UN proper shipping name DIISOBUTYL KETONE

14.3. Transport hazard class(es) 3 14.4. Packing group III

**14.5. Environmental hazards**No hazards identified

14.6. Special precautions for user No special precautions required.

14.7. Maritime transport in bulk Not applicable, packaged goods according to IMO instruments

## **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)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
Diisobutylketone	108-83-8	203-620-1	ı	ı	X	X	KE-10907	Χ	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Diisobutylketone	108-83-8	Х	ACTIVE	X	-	X	Х	X

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The Dimension Line Rational Control of the Control

Legend: X - Listed '-' - Not Listed

KECL - NIER number or KE number (http://ncis.nier.go.kr/en/main.do)

Authorisation/Restrictions according to EU REACH

Not applicable

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	Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	J	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Ī	Diisobutylketone	108-83-8	=	-	-

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

Component	CAS No	Seveso III Directive (2012/18/EC) -	Seveso III Directive (2012/18/EC) -
		Qualifying Quantities for Major Accident	Qualifying Quantities for Safety Report
		Notification	Requirements
Diisobutylketone	108-83-8	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
Diisobutylketone	WGK1	

Component	France - INRS (Tables of occupational diseases)
Diisobutylketone	Tableaux des maladies professionnelles (TMP) - RG 84

#### 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

H335 - May cause respiratory irritation

H226 - Flammable liquid and vapor

Inventory

Substances List

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CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances IECSC - Chinese Inventory of Existing Chemical Substances

**KECL** - 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 Dangerous Goods by Road

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

Key literature references and sources for data

https://echa.europa.eu/information-on-chemicals

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

**Training Advice** 

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit

First aid for chemical exposure, including the use of eye wash and safety showers.

Chemical incident response training.

Fire prevention and fighting, identifying hazards and risks, static electricity, explosive atmospheres posed by vapours and dusts.

Health, Safety and Environmental Department **Prepared By** 

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**Revision Summary** New emergency telephone response service provider.

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** 

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

TSCA - United States Toxic Substances Control Act Section 8(b)

**ENCS** - Japanese Existing and New Chemical Substances

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

Ships

ATE - Acute Toxicity Estimate VOC - (Volatile Organic Compound)