

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

1.1. Product identifier

Product Description: 1,5-Hexadiyne, 50% in pentane
Cat No. : **18720**
Molecular Formula HC#CCH₂ CH₂ C#CH

Unique Formula Identifier (UFI) **82JG-Q6S5-5X0W-XNM5**

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

Recommended Use Laboratory chemicals.
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

Poison Centre - Emergency information services
Ireland : National Poisons Information Centre (NPIC) -
01 809 2166 (8am-10pm, 7 days a week)
Malta : +356 2395 2000
Cyprus : +357 2240 5611

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

Flammable liquids

Category 2 (H225)

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Health hazards

Aspiration Toxicity
Skin Corrosion/Irritation
Serious Eye Damage/Eye Irritation
Specific target organ toxicity - (single exposure)

Category 1 (H304)
Category 2 (H315)
Category 2 (H319)
Category 3 (H336)

Environmental hazards

Chronic aquatic toxicity

Category 2 (H411)

Full text of Hazard Statements: see section 16

2.2. Label elements



Signal Word

Danger

Hazard Statements

H225 - Highly flammable liquid and vapor
H304 - May be fatal if swallowed and enters airways
H315 - Causes skin irritation
H319 - Causes serious eye irritation
H336 - May cause drowsiness or dizziness
H411 - Toxic to aquatic life with long lasting effects
EUH066 - Repeated exposure may cause skin dryness or cracking

Precautionary Statements

P301 + P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician
P331 - Do NOT induce vomiting
P264 - Wash face, hands and any exposed skin thoroughly after handling
P337 + P313 - If eye irritation persists: Get medical advice/attention
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing
P280 - Wear protective gloves/protective clothing/eye protection/face protection
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

This product does not contain any known or suspected endocrine disruptors

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.2. Mixtures

Component	CAS No	EC No	Weight %	CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
n-Pentane	109-66-0	EEC No. 203-692-4	50	Flam. Liq. 2 (H225)

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				Asp. Tox. 1 (H304) STOT SE 3 (H336) Aquatic Chronic 2 (H411) (EUH066)
1,5-Hexadiyne	628-16-0	EEC No. 211-029-5	50	Flam. Liq. 2 (H225) Asp. Tox. 1 (H304) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319)

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. 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

Difficulty in breathing. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting

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

Notes to Physician	Treat symptomatically.
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SECTION 5: FIREFIGHTING MEASURES

5.1. Extinguishing media

Suitable Extinguishing Media

Carbon dioxide (CO₂). Powder. Water spray. In case of major fire and large quantities: Evacuate area. Fight fire remotely due to the risk of explosion. 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

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

Hazardous Combustion Products

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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.

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

Do not flush into surface water or sanitary sewer system.

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 container tightly closed in a dry and well-ventilated place. Keep away from heat, sparks and flame.

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

Class 3

7.3. Specific end use(s)

Use in laboratories

SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1. Control parameters

Exposure limits

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List source(s): **EU** - Commission Directive (EU) 2019/1831 of 24 October 2019 establishing a fifth list of indicative occupational exposure limit values pursuant to Council Directive 98/24/EC and amending Commission Directive 2000/39/EC **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
n-Pentane	STEL: 1800 ppm 15 min STEL: 5400 mg/m ³ 15 min TWA: 600 ppm 8 hr TWA: 1800 mg/m ³ 8 hr	TWA: 1000 ppm (8hr) TWA: 3000 mg/m ³ (8hr)	TWA: 1000 ppm 8 hr. STEL: 3000 ppm 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)
n-Pentane 109-66-0 (50)				DNEL = 432mg/kg bw/day

Component	Acute effects local (Inhalation)	Acute effects systemic (Inhalation)	Chronic effects local (Inhalation)	Chronic effects systemic (Inhalation)
n-Pentane 109-66-0 (50)				DNEL = 3000mg/m ³

Predicted No Effect Concentration (PNEC)

See values below.

Component	Fresh water	Fresh water sediment	Water Intermittent	Microorganisms in sewage treatment	Soil (Agriculture)
n-Pentane 109-66-0 (50)	PNEC = 230µg/L	PNEC = 1.2mg/kg sediment dw	PNEC = 880µg/L	PNEC = 3600µg/L	PNEC = 0.55mg/kg soil dw

Component	Marine water	Marine water sediment	Marine water intermittent	Food chain	Air
n-Pentane 109-66-0 (50)	PNEC = 230µg/L	PNEC = 1.2mg/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

Goggles (European standard - EN 166)

Hand Protection

Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	480 minutes	0.4 mm	EN 374	(minimum requirement)
Skin and body protection		Long sleeved clothing.		

Inspect gloves before use.

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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 compatibility, 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.

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

Large scale/emergency use

In case of insufficient ventilation, wear suitable respiratory equipment

Recommended Filter type: Multi-purpose/ABEK 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.

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

Environmental exposure controls

Prevent product from entering drains. Do not allow material to contaminate ground water system.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Physical State	Liquid	
Appearance	Colorless to yellow	
Odor	No information available	
Odor Threshold	No data available	
Melting Point/Range	No data available	
Softening Point	No data available	
Boiling Point/Range	No information available	
Flammability (liquid)	Highly flammable	On basis of test data
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Flash Point	-2 °C / 28.4 °F	Method - No information available
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
pH	No information available	
Viscosity	No data available	
Water Solubility	Immiscible	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Component	log Pow	
n-Pentane	3.45	
Vapor Pressure	No data available	
Density / Specific Gravity	0.805 g/cm3	@ 20 °C
Bulk Density	Not applicable	Liquid
Vapor Density	No data available	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	

9.2. Other information

Molecular Formula	HC#CCH2 CH2 C#CH
Molecular Weight	78.11
Explosive Properties	Vapors may form explosive mixtures with air

SECTION 10: STABILITY AND REACTIVITY

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10.1. Reactivity

None known, based on information available

10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

Hazardous Polymerization

No information available.

Hazardous Reactions

None under normal processing.

10.4. Conditions to avoid

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

10.5. Incompatible materials

Oxidizing agent.

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;

Oral

Based on available data, the classification criteria are not met

Dermal

Based on available data, the classification criteria are not met

Inhalation

Based on available data, the classification criteria are not met

Toxicology data for the components

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
n-Pentane	> 2000 mg/kg (Rat)	3000 mg/kg (Rabbit)	364 g/m ³ (Rat) 4 h

(b) skin corrosion/irritation;

Category 2

(c) serious eye damage/irritation;

Category 2

(d) respiratory or skin sensitization;

Respiratory

No data available

Skin

No data available

(e) germ cell mutagenicity;

No data available

(f) carcinogenicity;

No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity;

No data available

(h) STOT-single exposure;

Category 3

Results / Target organs

Central nervous system (CNS).

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(i) STOT-repeated exposure; No data available
Target Organs No information available.

(j) aspiration hazard; Category 1

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

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

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

Component	Freshwater Fish	Water Flea	Freshwater Algae
n-Pentane	LC50: = 9.99 mg/L, 96h (Lepomis macrochirus) LC50: = 11.59 mg/L, 96h (Pimephales promelas) LC50: = 9.87 mg/L, 96h (Oncorhynchus mykiss)	EC50: = 9.74 mg/L, 48h (Daphnia magna)	

12.2. Persistence and degradability

Persistence Immiscible with water.
Degradation in sewage treatment plant Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.

12.3. Bioaccumulative potential May have some potential to bioaccumulate

Component	log Pow	Bioconcentration factor (BCF)
n-Pentane	3.45	No data available

12.4. Mobility in soil Spillage unlikely to penetrate soil The product is insoluble and floats on water Is not likely mobile in the environment due its low water solubility.

12.5. Results of PBT and vPvB assessment No data available for assessment.

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 This product does not contain any known or suspected substance
Ozone Depletion Potential This product does not contain any known or suspected substance

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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.

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

Do not flush to sewer. Waste codes should be assigned by the user based on the 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

UN3295

14.2. UN proper shipping name

Hydrocarbons, liquid, n.o.s.

Technical Shipping Name

(1,5-Hexadiyne 50%, Pentane)

14.3. Transport hazard class(es)

3

14.4. Packing group

II

ADR

14.1. UN number

UN3295

14.2. UN proper shipping name

Hydrocarbons, liquid, n.o.s.

Technical Shipping Name

(1,5-Hexadiyne 50%, Pentane)

14.3. Transport hazard class(es)

3

14.4. Packing group

II

IATA

14.1. UN number

UN3295

14.2. UN proper shipping name

Hydrocarbons, liquid, n.o.s.

Technical Shipping Name

(1,5-Hexadiyne 50%, Pentane)

14.3. Transport hazard class(es)

3

14.4. Packing group

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

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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
n-Pentane	109-66-0	203-692-4	-	-	X	X	KE-27968	X	X
1,5-Hexadiyne	628-16-0	211-029-5	-	-	-	-	KE-18535	-	-

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
n-Pentane	109-66-0	X	ACTIVE	X	-	X	X	X
1,5-Hexadiyne	628-16-0	X	ACTIVE	-	X	-	-	-

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

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
n-Pentane	109-66-0	-	-	-
1,5-Hexadiyne	628-16-0	-	-	-

Seveso III Directive (2012/18/EC)

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements
n-Pentane	109-66-0	Not applicable	Not applicable
1,5-Hexadiyne	628-16-0	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 .

Take note of Directive 2000/39/EC establishing a first list of indicative occupational exposure limit values

National Regulations

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

WGK Classification

Water endangering class = 2 (self classification)

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

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

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Component	Switzerland - Ordinance on the Reduction of Risk from handling of hazardous substances preparation (SR 814.81)	Switzerland - Ordinance on Incentive Taxes on Volatile Organic Compounds (OVOC)	Switzerland - Ordinance of the Rotterdam Convention on the Prior Informed Consent Procedure
n-Pentane 109-66-0 (50)	Prohibited and Restricted Substances	Group I	

15.2. Chemical safety assessment

Chemical Safety Assessment/Reports (CSA/CSR) are not required for mixtures

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
H319 - Causes serious eye irritation
H336 - May cause drowsiness or dizziness
H411 - Toxic to aquatic life with long lasting effects
EUH066 - Repeated exposure may cause skin dryness or cracking
H225 - Highly flammable liquid and vapor

Legend

CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical 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

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

DSL/NDL - Canadian Domestic Substances List/Non-Domestic Substances List

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

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

TWA - Time Weighted Average

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

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, Chemadviser - LOLI, Merck index, RTECS

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)

Classification and procedure used to derive the classification for mixtures according to Regulation (EC) 1272/2008 [CLP]:

Physical hazards On basis of test data

Health Hazards Calculation method

Environmental hazards Calculation method

Training Advice

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

Prepared By

Health, Safety and Environmental Department

Revision Date

17-Mar-2024

Revision Summary

New emergency telephone response service provider.

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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