

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

1.1. Product identifier

Product Description:	<u>2,4-Pentanedione</u>
Cat No. :	A14117
Synonyms	Acetylacetone
Index No	606-029-00-0
CAS No	123-54-6
EC No	204-634-0
Molecular Formula	C5 H8 O2
REACH registration number	-

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

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 3 (H226)

SAFETY DATA SHEET

2,4-Pentanedione

Revision Date 02-Feb-2024

Health hazards

Acute oral toxicity
Acute dermal toxicity
Acute Inhalation Toxicity - Vapors

Category 4 (H302)
Category 3 (H311)
Category 3 (H331)

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

Danger

Hazard Statements

H226 - Flammable liquid and vapor
H302 - Harmful if swallowed
H311 + H331 - Toxic in contact with skin or if inhaled

Precautionary Statements

P280 - Wear protective gloves/protective clothing/eye protection/face protection
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing
P311 - Call a POISON CENTER or doctor/physician
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)

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
2,4-Pentanedione	123-54-6	204-634-0	>95	Flam. Liq. 3 (H226) Acute Tox. 4 (H302) Acute Tox. 3 (H311) Acute Tox. 3 (H331)

REACH registration number

-

SAFETY DATA SHEET

2,4-Pentanedione

Revision Date 02-Feb-2024

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of first aid measures

General Advice	Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.
Eye Contact	In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice.
Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.
Ingestion	Do NOT induce vomiting. Call a physician or poison control center immediately.
Inhalation	Remove to fresh air. If breathing is difficult, give oxygen. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required.
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 (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

Water may be ineffective. Do not use a solid water stream as it may scatter and spread fire.

5.2. Special hazards arising from the substance or mixture

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

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. Thermal decomposition can lead to release of irritating gases and vapors.

SECTION 6: ACCIDENTAL RELEASE MEASURES

6.1. Personal precautions, protective equipment and emergency procedures

SAFETY DATA SHEET

2,4-Pentanedione

Revision Date 02-Feb-2024

Use personal protective equipment as required. Ensure adequate ventilation. Keep people away from and upwind of spill/leak. Evacuate personnel to safe areas. Remove all sources of ignition. Take precautionary measures against static discharges.

6.2. Environmental precautions

Should not be released into the environment. Do not flush into surface water or sanitary sewer system. 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. Take precautionary measures against static discharges.

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. Do not get in eyes, on skin, or on clothing. Use only under a chemical fume hood. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Take precautionary measures against static discharges. Use spark-proof tools and explosion-proof equipment.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice.

7.2. Conditions for safe storage, including any incompatibilities

Keep containers tightly closed in a dry, cool and well-ventilated place. Keep away from heat, sparks and flame. Flammables area.

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):

Component	The United Kingdom	European Union	Ireland
2,4-Pentanedione			TWA: 25 ppm 8 hr. STEL: 75 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)

SAFETY DATA SHEET

2,4-Pentanedione

Revision Date 02-Feb-2024

See table for values

Component	Acute effects local (Dermal)	Acute effects systemic (Dermal)	Chronic effects local (Dermal)	Chronic effects systemic (Dermal)
2,4-Pentanedione 123-54-6 (>95)				DNEL = 12mg/kg bw/day

Component	Acute effects local (Inhalation)	Acute effects systemic (Inhalation)	Chronic effects local (Inhalation)	Chronic effects systemic (Inhalation)
2,4-Pentanedione 123-54-6 (>95)				DNEL = 84mg/m ³

Predicted No Effect Concentration (PNEC)

See values below.

Component	Fresh water	Fresh water sediment	Water Intermittent	Microorganisms in sewage treatment	Soil (Agriculture)
2,4-Pentanedione 123-54-6 (>95)	PNEC = 0.2mg/L	PNEC = 1.909mg/kg sediment dw	PNEC = 0.26mg/L	PNEC = 1.32mg/L	PNEC = 0.19323mg/kg soil dw

Component	Marine water	Marine water sediment	Marine water intermittent	Food chain	Air
2,4-Pentanedione 123-54-6 (>95)	PNEC = 0.02mg/L	PNEC = 0.1909mg/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 Viton (R)	See manufacturers recommendations	-	EN 374	(minimum requirement)

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 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

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

SAFETY DATA SHEET

2,4-Pentanedione

Revision Date 02-Feb-2024

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 141

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

Environmental exposure controls Prevent product from entering drains.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Physical State	Liquid	
Appearance	Colorless	
Odor	pungent	
Odor Threshold	No data available	
Melting Point/Range	-23 °C / -9.4 °F	
Softening Point	No data available	
Boiling Point/Range	133 - 135 °C / 271.4 - 275 °F	@ 760 mmHg
Flammability (liquid)	Flammable	On basis of test data
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	Lower 2.4 Upper 11.4	
Flash Point	35.5 °C / 95.9 °F	Method - EU guideline A.9 / 1.6.3.2 / Abel method / ISO 13736
Autoignition Temperature	350 °C / 662 °F	
Decomposition Temperature	No data available	
pH	6 @ 20°C	200 g/l aq.sol
Viscosity	No data available	
Water Solubility	160 g/L (20°C)	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Component	log Pow	
2,4-Pentanedione	0.68	
Vapor Pressure	No data available	
Density / Specific Gravity	0.975	
Bulk Density	Not applicable	Liquid
Vapor Density	No data available	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	

9.2. Other information

Molecular Formula	C5 H8 O2
Molecular Weight	100.12
Explosive Properties	explosive air/vapour mixtures possible

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity

No

10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

SAFETY DATA SHEET

2,4-Pentanedione

Revision Date 02-Feb-2024

Hazardous Polymerization Hazardous Reactions

Hazardous polymerization does not occur.
None under normal processing.

10.4. Conditions to avoid

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

10.5. Incompatible materials

Acids. Strong oxidizing agents. oxygen. Metals.

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 Category 4
Dermal Category 3
Inhalation Category 3

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
2,4-Pentanedione	570-760 mg/kg (Rat)	810 µL/kg (Rabbit)	1224 ppm (Rat) 4 h

(b) skin corrosion/irritation; No data available

(c) serious eye damage/irritation; No data available

(d) respiratory or skin sensitization;

Respiratory No data available
Skin No data available

(e) germ cell mutagenicity;

Mutagenic effects have occurred in experimental animals

(f) carcinogenicity;

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; Reproductive Effects

Experiments have shown reproductive toxicity effects on laboratory animals.

(h) STOT-single exposure;

No data available

(i) STOT-repeated exposure;

No data available

Target Organs

No information available.

(j) aspiration hazard;

No data available

Other Adverse Effects

See actual entry in RTECS for complete information

SAFETY DATA SHEET

2,4-Pentanedione

Revision Date 02-Feb-2024

Symptoms / effects, both acute and delayed Symptoms of overexposure may be 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

Do not empty into drains. Contains a substance which is: Harmful to aquatic organisms. The product contains following substances which are hazardous for the environment.

Component	Freshwater Fish	Water Flea	Freshwater Algae
2,4-Pentanedione	LC50: 50.3 - 71.8 mg/L, 96h flow-through (Lepomis macrochirus) LC50: 64.1 - 80.1 mg/L, 96h flow-through (Oncorhynchus mykiss) LC50: 98.3 - 110 mg/L, 96h flow-through (Pimephales promelas)	EC50: = 34.4 mg/L, 48h (Daphnia magna)	

Component	Microtox	M-Factor
2,4-Pentanedione	EC50 = 1050 mg/L 5 min	

12.2. Persistence and degradability

Persistence

Expected to be biodegradable

Degradation in sewage treatment plant

Soluble in water, Persistence is unlikely, based on information available.

Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.

12.3. Bioaccumulative potential

Bioaccumulation is unlikely

Component	log Pow	Bioconcentration factor (BCF)
2,4-Pentanedione	0.68	No data available

12.4. Mobility in soil

The product is water soluble, and may spread in water systems. Will likely be mobile in the environment due to its water solubility. Highly mobile in soils

12.5. Results of PBT and vPvB assessment

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

SAFETY DATA SHEET

2,4-Pentanedione

Revision Date 02-Feb-2024

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.

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

14.1. UN number	UN2310
14.2. UN proper shipping name	PENTANE-2,4-DIONE
14.3. Transport hazard class(es)	3
Subsidiary Hazard Class	6.1
14.4. Packing group	III

ADR

14.1. UN number	UN2310
14.2. UN proper shipping name	PENTANE-2,4-DIONE
14.3. Transport hazard class(es)	3
Subsidiary Hazard Class	6.1
14.4. Packing group	III

IATA

14.1. UN number	UN2310
14.2. UN proper shipping name	PENTANE-2,4-DIONE
14.3. Transport hazard class(es)	3
Subsidiary Hazard Class	6.1
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 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)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
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SAFETY DATA SHEET

2,4-Pentanedione

Revision Date 02-Feb-2024

2,4-Pentanedione	123-54-6	204-634-0	-	-	X	X	KE-27993	X	X
Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS	
2,4-Pentanedione	123-54-6	X	ACTIVE	X	-	X	X	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)
2,4-Pentanedione	123-54-6	-	-	-

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
2,4-Pentanedione	123-54-6	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
2,4-Pentanedione	WGK1	

Component	France - INRS (Tables of occupational diseases)
2,4-Pentanedione	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

SAFETY DATA SHEET

2,4-Pentanedione

Revision Date 02-Feb-2024

H226 - Flammable liquid and vapor
H302 - Harmful if swallowed
H311 - Toxic in contact with skin
H331 - Toxic if inhaled

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, Chemadvisor - 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)

Training Advice

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

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

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

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

Chemical incident response training.

Prepared By

Health, Safety and Environmental Department

Creation Date

22-Sep-2009

Revision Date

02-Feb-2024

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