2,3-Pentanedione

AN ILLOVO SUGAR AFRICA COMPANY

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

1.1 Product identifier

Chemical name	2,3-Pentanedione		
Synonyms	2,3-Pentadione, Acetyl propionyl, Pentane-2,3-dione.		
Formula	$C_5H_8O_2$		
Molecular mass	100.12	**FL-No.**	07.060
CAS-No.	600-14-6	**FEMA-No.**	2841
EC-No.	209-984-8	**Annex VI-No.**	–
Registration number	The substance does not require registration as a food additive in foodstuffs, a flavouring in foodstuffs, an additive in feeding stuffs, in animal nutrition according to title II of the REACH Regulation.		

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

Relevant identified uses of the substance or mixture

Flavouring agent, intermediate for the manufacture of other flavours.

Uses advised against

None.

1.3 Details of the supplier of the safety data sheet

Manufacturer	Illovo Sugar (South Africa) (Pty) Ltd
Address	1 Nokwe Avenue Ridgeside Umhlanga Rocks South Africa 4320
Telephone number	+27 31 508 45 88
E-mail address	commercialdownstreamsds@illovo.co.za
Only representative	Otentic Customs BV
Address	Zeilmakerijweg 8, 4906 CW Oosterhout, The Netherlands
Telephone number	+31 162 48 80 50

1.4 Emergency telephone numbers

Emergency

– **Local South Africa**	0800 17 27 43	Rapid Spill Response
– **International**	+27 82 775 33 05	

Medical information

– **South Africa**	+27 824 910 160	Bloemfontein Poison Control and Medicine Information Centre
– **South Africa**	+27 861 555 777	Poisons Information Helpline of the Western Cape
– **United Kingdom**	844 892 0111	National Poisons Information Service

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

According to Regulation (EC) No. 1272/2008 (EU-GHS / CLP)

Hazard Classes / Hazard Class-, Category- and -Statement Codes

Flammable liquid	Flam. Liq. 2, H225
Specific target organ toxicity – repeated exposure	STOT RE 2, H373
Eye irritation	Eye Irrit. 2, H319
Skin irritation	Skin Irrit. 2, H315

For full text of Hazard statements: see subsection 2.2.

2.2 Label elements

According to Regulation (EC) No. 1272/2008 (EU-GHS / CLP)

Hazard pictograms

Signal word Danger

Hazard statements

H225	Highly flammable liquid and vapour.
H373	May cause damage to respiratory system through prolonged or repeated exposure by inhalation.
H319	Causes serious eye irritation.
H315	Causes skin irritation.

Precautionary statements

P210 *	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P240	Ground / bond container and receiving equipment.
P241	Use explosion-proof electrical ventilating- / lighting- / process equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P260 *	Do not breathe vapours.
P280 *	Wear protective gloves / protective clothing / eye protection.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P305 + P351 + P338 *	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337 + P313	If eye irritation persists: Get medical advice / attention.
P363	Wash contaminated clothing before reuse.
P403 + P233 *	Store in a well-ventilated place. Keep container tightly closed.
P501	Dispose of contents / container to a specialised processing facility for disposal in accordance with local / regional regulations.

* on label

2.3 Other hazards

2,3-Pentanedione does not meet the criteria for PBT or vPvB according to Regulation 1907/2006.

SECTION 3: Composition / information on ingredients

3.1 Substances

Main constituent	Identity		Percentage
2,3-Pentanedione	CAS-No.	600-14-6	>98 %
	EC-No.	209-984-8	

Classified impurities or stabilizers

None

SECTION 4: First aid measures

4.1 Description of first aid measures

Inhalation
Fresh air, rest, half upright position. Get medical advice / attention if you feel unwell.

Skin contact
Remove contaminated clothes, rinse skin with water or shower. If skin irritation occurs: get medical advice / attention.

Eye contact
First rinse with plenty of water (remove lenses if possible). If eye irritation persists: get medical advice / attention.

Ingestion
Rinse mouth. Get medical advice / attention if you feel unwell.

4.2 Most important symptoms and effects, both acute and delayed

Acute symptoms and effects from exposure

Redness and pain in the eyes. Redness of the skin.

Delayed symptoms and effects from exposure

Experimental inhalation studies with rats showed that 2,3-Pentanedione exposure produces identical respiratory pathology to that of Diacetyl.
Therefore Pentanedione may cause damage to lungs [obliterative bronchiolitis (OB)] through prolonged or repeated exposure by inhalation.
Symptoms of lung disease may include (but is not limited to) persistent dry cough, wheezing, shortness of breath upon exertion and fixed airways obstruction on spirometry.

4.3 Indication of any immediate medical attention and special treatment needed

Information on medical attendance

Not known.

Special means to provide treatment at the workplace

Not known.

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Powder, water spray, alcohol-resistant foam, carbon dioxide.

Unsuitable extinguishing media

Water jet, alcohol unstable foam.

5.2 Special hazards arising from the substance or mixture

Hazardous combustion products

May produce toxic fumes of carbon monoxide if burning.

Additional hazards

Brief exposure through inhalation to high concentrations may cause lung disease.
The vapour is heavier than air, spreads along the ground and distant ignition is possible.

5.3 Advice for fire-fighters

Protective actions

In case of fire: keep containers cool by spraying with water.
Retain contaminated extinguishing water; do not allow entering into the sewage system.
In the case of larger fires: Cordon affected area.

Special protective equipment

Self-contained respiratory protective device, full protective suit.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Information for non-emergency personnel

Eliminate all sources of ignition.
Use personal protective equipment to avoid any contamination of skin and eyes. Do not breathe vapours.
Indoor spills: Assure sufficient ventilation.
Outdoor spills: Stay up wind and keep out of low areas where vapour may accumulate and ignite.
Stop leak if this can be achieved without risk.
In the case of large quantities: Consider need for evacuation.

Information for emergency responders

For advice on personal protection clothing, see chapter 8.

6.2 Environmental precautions

Try to prevent the material from entering drains, water courses or soil.
Advise authorities if spillage has entered water course or sewer or has contaminated soil.

6.3 Methods and material for containment and cleaning up

Small spills: Allow to evaporate if it is safe to do so or contain and absorb using earth, sand or other inert material then transfer into suitable containers for recovery or disposal.
Large spills: Ventilate contaminated area thoroughly. Cover drains. Dike or dam in and vacuum up carefully. Wash away remainder with water.

6.4 Reference to other sections

See Section 8 for more detailed advice on personal protective equipment and section 13 on waste disposal.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Recommendations for safe handling

Use only in well ventilated areas and in a closed system.
Keep away from heat, sparks, open flames, hot surfaces and do not smoke.
Do not breathe vapours. Avoid contact with eyes, skin and clothing.
Take measures to prevent electrostatic charges, e.g. grounding when transferring/ filing.
Containers have to be properly labelled.

Advice on general occupational hygiene

Do not eat, drink and smoke in work areas.
Use fatty skin care products after repeated contact and washing hands.

7.2 Conditions for safe storage, including any incompatibilities

Precautions for safe storage and protection against incompatible substances

Store in a well-ventilated place. Keep containers tightly closed.
Keep away from oxidants, reducing agents, strong bases and strong acids.
Store away from sources of heat or ignition. Storage tanks should have equipotential electrical bonding and be earthed.
Beware of formation of explosive vapour-air mixtures in empty, uncleaned containers.

Protection against ambient influences

Protect against heat and solar radiation. Recommended storage temperature: 20 ºC.
The substance affects many synthetic materials; store only in original packing.
Suited materials for containers are: Pentanedione resistant plastics, mild steel, stainless steel.

Maintenance of the integrity of the substance

Not required.

7.3 Specific end use(s)

If used in food: comply with food safety regulation (HACCP).

8. EXPOSURE CONTROLS / PERSONAL PROTECTION

8.1 Control parameters

	Limit values				
	8 hours (TWA)		Short term (15 min.)		Notation
	mg/m^3	ppm	mg/m^3	ppm	
	n.d.		n.d.		

n.d. not determined

DNEL / DMEL values

No data available.

PNEC values

No data available.

8.2 Exposure controls

8.2.1 Appropriate engineering controls

Ventilation and local exhaust.

8.2.2 Individual protection measures, such as personal protective

a) Eye/face protection

Safety goggles (EN 166).

b) Skin protection

Hand protection	Gloves butyl rubber 0.7 mm	Breakthrough time > 8 hours (EN 374)
	Gloves nitrile rubber 0.4 mm	Breakthrough time > 30 minutes (EN 374)
	Gloves Viton 0.7 mm	Breakthrough time > 8 hours (EN 374)
Other	Protective clothing (EN 340/EN 14605).	

c) Respiratory protection

In case of insufficient local exhaust: filter respirator with filtertype A for organic vapours (EN 14387).

d) Thermal hazards

Not applicable.

8.2.3 Environmental exposure controls

Direct polluted air of the local exhaust ventilation out of the plant in a manner in accordance with environmental regulations.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Appearance	Clear yellow liquid
Odour	Buttery
Odour threshold (mg/m3)	Not available
pH (20% solution)	4
Melting point / freezing point (˚C)	– 52
Boiling point (˚C) at 1013 hPa	110 - 112
Flash point (˚C)	18 (tag closed cup)
Evaporation rate (ether=1)	Not available
Lower/upper explosive limits (vol%)	1.8 – 10.9

Vapour pressure at 20 ˚C (hPa)	28.5
Vapour density (air=1)	3.45
Relative density (water=1)	0.959
Solubility(ies)	
– **Solubility in water at 20 ˚C (g/l)**	60
– **Solubility in fat**	Good
Partition coefficient (log K octanol/water)	– 0.85
Auto-ignition temperature (˚C)	265
Decomposition temperature (˚C)	> 100
Viscosity at 25 ˚C (mPa.s)	Not available
Explosive properties	None
Oxidising properties	None

9.2 Other information

Miscibility with	Ethanol, ether, acetone.
Conductivity (pS/m)	Not available
Heat of combustion (kJ/kg)	Not available

SECTION 10: Stability and reactivity

10.1 Reactivity

Exothermic, partially violent reactions with oxidising agents, reducing agents, strong acids and bases possible.

10.2 Chemical stability

Stable at usual storage conditions. No stabilizers required.

10.3 Possibility of hazardous reactions

Excessive heat generation or splashes of hazardous substances with oxidising agents, reducing agents, strong bases and acids.

10.4 Conditions to avoid

Storage temperatures > 40 °C should be avoided (increase in pressure, deformation of the containers).
Avoid static discharge and sources of ignition (open flames, warm surfaces, sparks).

10.5 Incompatible materials

Strong oxidising agents and reducing agents, strong acids and bases.
The substance affects some plastics and various metals.

10.6 Hazardous decomposition products

Does not decompose when used for intended uses.

SECTION 11 Toxicological information

11.1 Information on toxicological effects

a) Acute toxicity

– ***Oral***	LD50 (rat)	3 000 mg/kg
– ***Dermal***	LD50 (rat)	>2 500 mg/kg
– ***Inhalation***	LC50 (rat, 4 hours)	Not available

b) Skin corrosion/irritation

The substance is irritating to skin.

c) Serious eye damage/irritation

The substance is irritating to eyes.

d) Respiratory or skin sensitisation

The result of available human data gave no evidence of sensitization by skin contact.

e) Germ cell mutagenicity

The substance does not induce gene mutation in bacteria in vitro.

f) Carcinogenicity

Not suspected of causing cancer.

g) Reproductive toxicity

No test data available.

h) Specific target organ toxicity – single exposure

Exposure at high levels could cause lowering of consciousness.

i) Specific target organ toxicity – repeated exposure

Because 2,3-Pentanedione share the same functional alpha-diketone group as Diacetyl, this substance may also share Diacetyl's mechanism of toxicity.
This possibility is confirmed by experimental inhalation studies with rats.
Therefore it is possible that intermittent and subchronic exposures to occupationally-relevant 2,3-Pentanedione concentrations causes lymphocytic bronchitis and bronchiolitis. Lymphocytic bronchitis is a precursor lesion to obliterative bronchiolitis (OB), which causes airway epithelial damage.

j) Aspiration hazard

No indication that the substance may pose aspiration toxicity.

k) Maximum levels of consumption

The maximum recommended 2,3-Pentanedione usage level in foodstuffs is 50 ppm in the finished product.

11.2 Likely routes of exposure

The substance may be absorbed into the body by inhalation of vapour or spray and after ingestion.

11.3 Delayed and immediate effects as well as chronic effects from short and long-term exposure

In case of lung disease: symptoms of lung disease may include (but is not limited to) persistent dry cough, wheezing, shortness of breath upon exertion and fixed airways obstruction on spirometry.
Even brief exposure through inhalation to high concentrations may cause OB.
The loss of pulmonary function associated with this illness is permanent.

SECTION 12: Ecological information

12.1 Toxicity

Aquatic toxicity

– ***Fish***

LC50 (96 hr)	46 - 100 mg/L
NOEC (96 hr)	No data available

– ***Aquatic invertebrates***

LC50 (48 hr)	> 100 mg/L (calculated)
NOEC (48 hr)	No data available

– ***Algae and cyanobacteria***

EC50 (17 hr)	220 mg/L
NOEC (96 hr)	No data available

Sediment toxicity

LC50 (96 hr)	No data available

Terrestrial toxicity

– ***Terrestrial arthropods*** No data available

– ***Other soil macro-organisms***

LC50 (48 hr)	No data available

– ***Terrestrial plants*** No data available

12.2 Persistence and degradability

Stability

– ***Hydrolysis***	Half-life (DT50 in water)	15 days
– ***Photolysis***	Half-life (DT50 in air)	8 days

Biodegradability

– ***Biodegradation in water***

Pentanedione is biodegradable in water (biodegradation probability 0.5 - 0.8).

– ***Biochemical oxygen demand***

BOD (5 days)	No data available
BOD (20 days)	No data available

12.3 Bioaccumulation potential

Aquatic bioaccumulation

BCF (based on a regressionderived equation). 3

The potential for bioconcentration in aquatic organism is low (log K_{ow} < 4 and BCF < 500).

12.4 Mobility in soil

Adsorption/desorption K_{oc} at 20 °C 1 (calculated)
Pentanedione is expected to have very high mobility in soil.

Volatilisation Henry's Law constant at 25 °C (in Pa m^3/mole) 0.26
Based upon the Henry's Law constant volatilization from moist soil surfaces is not expected.

12.5 Results of PBT and vPvB assessment

The substance does not meet the PBT and vPvB criteria according to annex XIII of Regulation (EC) No 1907/2006.

12.6 Other adverse effects

Low hazard to water (Water hazard class 1, WGK Germany)

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product disposal Recycling by distillation.
Removal to an authorized waste incinerator for solvents or as chemical waste in accordance with local regulations. Do not discharge wastewater into sewer.

Packaging disposal Uncleaned empty package have to be treated like the content. The labelling of uncleaned containers must not be removed.

Waste treatment-relevant information
European waste list (EURAL) 07 01 04

SECTION 14: Transport information

14.1 UN number	1224
14.2 UN proper shipping name	KETONES, LIQUID, N.O.S. (2,3-Pentanedione)
14.3 Transport hazard class(es)	3
14.4 Packing group	II

14.5 Environmental hazards

Marine pollutant (IMO/IMDG)	No
Hazards for tank vessels (ADN)	3+(N1, N2, N3, CMR, F or S)

14.6 Specials precautions for user

Classification code (ADR/RID/ADN)	F1
Risk labels (ADR/RID/ADN/IMDG/IATA)	3
Tunnel restriction code (ADR/RID)	(D/E)
Hazard Identification No. (ADR/RID)	33
Limited quantity (ADR/RID/ADN/IMDG/IATA)	1 L
Excepted quantity (ADR/RID/IATA)	E2
ERICard (ADR)	3-11
Emergency Schedules (IMDG)	
– **Fire schedule**	Alfa (F - E)
– **Spillage schedule**	Afa (S - D)

14.7 Transport in bulk according to Annex II of Marpol and the IBC Code

Ship type required (IMDG)	Not available
Pollution category (IMDG)	Not available

SECTION15: Regulatory information

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

Authorisations (REACH)
Not subject to Title VII of Regulation (EC) No 1907/2006.

Restrictions (REACH), SVHC
Annex XVII of Regulation (EC) No 1907/2006 is not applicable.
SVHC (Substances of Very High Concern) status: negative

Control of major-accident hazards (Seveso III)

Subject to Directive 2012/18/EU:	P5c FLAMMABLE LIQUIDS
Qualifying quantity column 2:	5 000 000 kg
Qualifying quantity column 3:	50 000 000 kg

List of flavouring substances

Approved as a flavouring agent (Regulation (EU) No 872/2012).

Other EU regulations Additional national regulations have to be observed.

15.2 Chemical safety assessment

A Chemical Safety Assessment has not been carried out for Pentanedione.

SECTION 16: Other information

16.1 Changes to the previous version

Previous version 19.3

Changes Change of logo and details of supplier; removal of the pre-registration number, change of the e-mail address and addition of the language code.

16.2 Abbreviations and acronyms

ADN	Transport of dangerous goods by inland waterways
ADR	Transport of dangerous goods by road
CAS	Chemical Abstracts Service (Division der American Chemical Society)
CLP	Classification, Labelling and Packaging
CSA	Chemical Safety Assessment
CSR	Chemical Safety Report
DNEL	Derived No Effect Level
DMEL	Derived Minimal Effect Level
EC50	Effect Concentration, 50 percent
EC-Number	EINECS-, ELINCS- or CLP-Number
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
ERICard	Emergency Response Intervention Card
GHS / CLP	Globally Harmonised System / Classification, Labelling and Packaging
IATA	Transport of dangerous goods by air
IMDG	Transport of dangerous goods by sea
IC50	Inhibitory Concentration, 50 percent
LC50	Lethal Concentration, 50 percent
LD50	Lethal Dose, 50 percent
NOAEC	No observed adverse effect concentration
NOAEL	No observed adverse effect level
NOEC	No observed adverse effect concentration
NOEL	No observed effect level
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
ppm	Parts per million
RID	Transport of dangerous goods by rail
TWA	Time Weighted Average
vPvB	very persistent and very bioaccumulative

16.3 Literature references and sources for data

Joint FAO/WHO Expert Committee on Food Additives;
Mosciano, Gerard P&F 22, No. 1, 57, (1997);
D.L. Morgan e.a., Inhalation toxicity of acetyl propionyl in rats and mice, 1492, The Toxicologist: Journal of the Society of Toxicology, Volume 114, (1), 316, 2010.
A.F. Hubbs e.a., Airway epithelial toxicity of the flavouring agent, 2,3-Pentanedione, The Toxicologist: Journal of the Society of Toxicology, Volume 114, (1), 319, 2010.
Database EPIWEB

16.4 Full text of Hazard statements which are not written out in full under Sections 2 to 15

None.