

ALFAAB20653

## 3-Hexyne-2,5-diol, (+/-) + meso

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

产品说明:  
 Product Description: 3-Hexyne-2,5-diol, (+/-) + meso  
 3-Hexyne-2,5-diol, (+/-) + meso

Cat No. : B20653  
 CAS No 3031-66-1  
 Molecular Formula C6H10O2

Supplier Avocado Research Chemicals Ltd.  
 (Part of Thermo Fisher Scientific)  
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 Lancashire, LA3 2XY,  
 United Kingdom  
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 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

E-mail address begel.sdsdesk@thermofisher.com

Recommended Use Laboratory chemicals.  
 Uses advised against No Information available

### SECTION 2. HAZARD IDENTIFICATION

**Physical State**  
 Low melting solid

**Appearance**  
 No information available

**Odor**  
 No information available

#### Emergency Overview

May cause an allergic skin reaction. Causes serious eye damage. Toxic if swallowed. Causes skin irritation. May cause damage to organs through prolonged or repeated exposure. Toxic to aquatic life with long lasting effects.

#### Classification of the substance or mixture

Acute Oral Toxicity	Category 3
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 1
Skin Sensitization	Category 1
Specific target organ toxicity - (repeated exposure)	Category 2
Chronic aquatic toxicity	Category 2

#### Label Elements



**Signal Word****Danger****Hazard Statements**

H315 - Causes skin irritation

H317 - May cause an allergic skin reaction

H301 - Toxic if swallowed

H318 - Causes serious eye damage

H373 - May cause damage to organs through prolonged or repeated exposure

H411 - Toxic to aquatic life with long lasting effects

**Precautionary Statements****Prevention**

P264 - Wash face, hands and any exposed skin thoroughly after handling

P270 - Do not eat, drink or smoke when using this product

P272 - Contaminated work clothing should not be allowed out of the workplace

P280 - Wear protective gloves/protective clothing/eye protection/face protection

**Response**

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

P310 - Immediately call a POISON CENTER or doctor

P330 - Rinse mouth

P362 + P364 - Take off contaminated clothing and wash it before reuse

**Storage**

P405 - Store locked up

**Disposal**

P501 - Dispose of contents/ container to an approved waste disposal plant

**Physical and Chemical Hazards**

None identified.

**Health Hazards**

Causes skin irritation. May cause an allergic skin reaction. Toxic if swallowed. May cause damage to organs through prolonged or repeated exposure.

**Environmental hazards**

Toxic to aquatic life with long lasting effects.

Toxic to terrestrial vertebrates. This product does not contain any known or suspected endocrine disruptors.

**SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

Component	CAS No	Weight %
3-Hexyne-2,5-diol	3031-66-1	<=100

**SECTION 4. FIRST AID MEASURES****Eye Contact**

Rinse thoroughly with plenty of water for at least 15 minutes, lifting lower and upper eyelids. Consult a physician.

**Skin Contact**

Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes.

**Inhalation**

Remove to fresh air.

**Ingestion**

Clean mouth with water and drink afterwards plenty of water.

**Most important symptoms and effects**

Causes eye burns. May cause allergic skin reaction. Causes severe eye damage. Symptoms of allergic reaction may include rash,

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itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing

**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.

**Notes to Physician**

Treat symptomatically.

**SECTION 5. FIRE-FIGHTING MEASURES****Suitable Extinguishing Media**

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

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

No information available.

**Specific Hazards Arising from the Chemical**

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

**Protective Equipment and Precautions 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****Personal Precautions**

Ensure adequate ventilation.

**Environmental Precautions**

Do not flush into surface water or sanitary sewer system.

Refer to protective measures listed in Sections 8 and 13.

**SECTION 7. HANDLING AND STORAGE****Handling**

Ensure adequate ventilation.

**Storage**

Keep container tightly closed in a dry and well-ventilated place.

**Specific Use(s)**

Use in laboratories

**SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION****Control Parameters****Exposure Controls****Engineering Measures**

Ensure that eyewash stations and safety showers are close to the workstation location. Wherever possible, engineering control

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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	See manufacturers	-	EN 374	(minimum requirement)
Neoprene	recommendations			
Natural rubber				
PVC				

Inspect gloves before use.

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

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

Remove gloves with care avoiding skin contamination.

**Skin and body protection** Long sleeved clothing

**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  
**Recommended Filter type:** Particulates filter conforming to EN 143

**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:-** Particle filtering: EN149:2001  
When RPE is used a face piece Fit Test should be conducted

**Hygiene Measures** Handle in accordance with good industrial hygiene and safety practice.

**Environmental exposure controls** Prevent product from entering drains. Do not allow material to contaminate ground water system.

## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

<b>Appearance</b>		
<b>Physical State</b>	Low melting solid	
<b>Odor</b>	No information available	
<b>Odor Threshold</b>	No data available	
<b>pH</b>	Not applicable	
<b>Melting Point/Range</b>	No data available	
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	No data available	
<b>Flash Point</b>	123 °C / 253.4 °F	<b>Method -</b> No information available
<b>Evaporation Rate</b>	No data available	
<b>Flammability (solid,gas)</b>	No information available	
<b>Explosion Limits</b>	No data available	
<b>Vapor Pressure</b>	No data available	
<b>Vapor Density</b>	No data available	(Air = 1.0)
<b>Specific Gravity / Density</b>	1.01	

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Bulk Density	No data available
Water Solubility	No information available
Solubility in other solvents	No information available
Partition Coefficient (n-octanol/water)	
Autoignition Temperature	No data available
Decomposition Temperature	No data available
Viscosity	No data available
Explosive Properties	No information available
Oxidizing Properties	No information available

Molecular Formula	C6H10O2
Molecular Weight	114.15

## SECTION 10. STABILITY AND REACTIVITY

Stability	Stable under normal conditions.
Hazardous Reactions	No information available.
Hazardous Polymerization	No information available.
Conditions to Avoid	None known.
Materials to avoid	No information available.

Hazardous Decomposition Products Carbon oxides.

## SECTION 11. TOXICOLOGICAL INFORMATION

## Product Information

## (a) acute toxicity;

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
3-Hexyne-2,5-diol		LD50 > 2000 mg/kg ( Rat )	

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 1

## (d) respiratory or skin sensitization;

Respiratory	No data available
Skin	Category 1

May cause sensitization by skin contact

(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; No data available

(i) STOT-repeated exposure;	Category 2
Target Organs	No information available.
(j) aspiration hazard;	No data available
Symptoms / effects, both acute and delayed	Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing

**SECTION 12. ECOLOGICAL INFORMATION**

Ecotoxicity effects	Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment. The product contains following substances which are hazardous for the environment.
Persistence and Degradability Degradation in sewage treatment plant	No information available Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.
Bioaccumulative Potential	No information available
Mobility in soil	No information available
Endocrine Disruptor Information Persistent Organic Pollutant Ozone Depletion Potential	This product does not contain any known or suspected endocrine disruptors This product does not contain any known or suspected substance This product does not contain any known or suspected substance

**SECTION 13. DISPOSAL CONSIDERATIONS**

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.
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. Do not empty into drains. Do not let this chemical enter the environment.

**SECTION 14. TRANSPORT INFORMATION****Road and Rail Transport**

UN-No	UN2811
Proper Shipping Name	TOXIC SOLID, ORGANIC, N.O.S.
Technical Shipping Name	3-Hexyne-2,5-diol
Hazard Class	6.1
Packing Group	III

**IMDG/IMO**

UN-No	UN2811
Proper Shipping Name	TOXIC SOLID, ORGANIC, N.O.S.

**SAFETY DATA SHEET****3-Hexyne-2,5-diol, (+/-) + meso**

**Technical Shipping Name** 3-Hexyne-2,5-diol  
**Hazard Class** 6.1  
**Packing Group** III

**IATA**

**UN-No** UN2811  
**Proper Shipping Name** TOXIC SOLID, ORGANIC, N.O.S.  
**Technical Shipping Name** 3-Hexyne-2,5-diol  
**Hazard Class** 6.1  
**Packing Group** III

**Special Precautions for User** No special precautions required

**SECTION 15. REGULATORY INFORMATION****International Inventories**

China, X = listed, Australia, U.S.A. (TSCA), Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Australia (AICS), Korea (KECL), China (IECSC), Japan (ENCS), Philippines (PICCS), Taiwan (TCSI), Japan (ISHL), New Zealand (NZIoC), Japan (ISHL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
3-Hexyne-2,5-diol	-	-	X	X	221-209-5	X	X	X	X	X	X	KE-19941

**National Regulations****SECTION 16. OTHER INFORMATION**

**Prepared By** Health, Safety and Environmental Department  
**Creation Date** 26-Oct-2022  
**Revision Date** 13-May-2024  
**Revision Summary** New emergency telephone response service provider.

**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.

**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/NDSL** - 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

**TWA** - Time Weighted Average

**IARC** - International Agency for Research on Cancer

**PNEC** - Predicted No Effect Concentration

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**RPE** - Respiratory Protective Equipment  
**LC50** - Lethal Concentration 50%  
**NOEC** - No Observed Effect Concentration  
**PBT** - Persistent, Bioaccumulative, Toxic

**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

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road

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

**BCF** - Bioconcentration factor

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

**MARPOL** - International Convention for the Prevention of Pollution from Ships

**ATE** - Acute Toxicity Estimate

**VOC** - (Volatile Organic Compound)

**Key literature references and sources for data**

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

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

**Disclaimer**

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**End of Safety Data Sheet**