

ALFAAA10624

4'-Isobutylacetophenone

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

产品说明: 4'-异丁基苯乙酮
Product Description: 4'-Isobutylacetophenone

Cat No. : A10624
CAS No 38861-78-8
Molecular Formula C12 H16 O

Supplier Avocado Research Chemicals Ltd.
(Part of Thermo Fisher Scientific)
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Recommended Use Laboratory chemicals.
Uses advised against No Information available

SECTION 2. HAZARD IDENTIFICATION

Physical State
Liquid

Appearance
No information available

Odor
No information available

Emergency Overview
Flammable liquid and vapor. May cause an allergic skin reaction. Toxic to aquatic life with long lasting effects.

Classification of the substance or mixture

Flammable liquids.	Category 3
Skin Sensitization	Category 1
Chronic aquatic toxicity	Category 2

Label Elements



Signal Word

Warning

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Hazard Statements

H226 - Flammable liquid and vapor
H317 - May cause an allergic skin reaction
H411 - Toxic to aquatic life with long lasting effects

Precautionary Statements**Prevention**

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking
P233 - Keep container tightly closed
P240 - Ground and bond container and receiving equipment
P243 - Take action to prevent static discharges
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray
P242 - Use non-sparking tools
P280 - Wear protective gloves/protective clothing/eye protection/face protection
P272 - Contaminated work clothing should not be allowed out of the workplace

Response

P333 + P313 - If skin irritation or rash occurs: Get medical advice/attention
P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower
P370 + P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish
P362 + P364 - Take off contaminated clothing and wash it before reuse

Storage

P403 + P235 - Store in a well-ventilated place. Keep cool

Disposal

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

Physical and Chemical Hazards

Flammable liquid. Vapors may cause flash fire or explosion.

Health Hazards

May cause an allergic skin reaction.

Environmental hazards

Toxic to aquatic life with long lasting effects. .

This product does not contain any known or suspected endocrine disruptors.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Component	CAS No	Weight %
Ethanone, 1-[4-(2-methylpropyl)phenyl]-	38861-78-8	>95

SECTION 4. FIRST AID MEASURES**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. Get medical attention.

Inhalation

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

Ingestion

Do NOT induce vomiting. Get medical attention.

Most important symptoms and effects

Difficulty in breathing. May cause allergic skin reaction. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting: 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

Self-Protection of the First Aider

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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**

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

No information available.

Specific Hazards Arising from the Chemical

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

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

SECTION 6. ACCIDENTAL RELEASE MEASURES**Personal Precautions**

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

Environmental Precautions

Do not flush into surface water or sanitary sewer system.

Methods for Containment and Clean 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.

Refer to protective measures listed in Sections 8 and 13.

SECTION 7. HANDLING AND STORAGE**Handling**

Wear personal protective equipment/face protection. 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. Use spark-proof tools and explosion-proof equipment. Take precautionary measures against static discharges.

Storage

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

Specific Use(s)

Use in laboratories

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION**Control Parameters**

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Monitoring methods

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS70 General methods for sampling airborne gases and vapours MDHS 88 Volatile organic compounds in air. Laboratory method using diffusive samplers, solvent desorption and gas chromatography MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

Exposure Controls**Engineering Measures**

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

Skin and body protection	Wear appropriate protective gloves and clothing to prevent skin exposure
Respiratory Protection	No protective equipment is needed under normal use conditions.
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
Small scale/Laboratory use	Maintain adequate ventilation

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

Appearance
Physical State

Liquid

Odor
Odor Threshold
pH
Melting Point/Range
Softening Point
Boiling Point/Range
Flash Point

No information available
No data available
No information available
No data available
No data available
107 °C / 224.6 °F
54 °C / 129.2 °F

@ 2 mmHg
Method - No information available

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Evaporation Rate	No data available	
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Vapor Pressure	No data available	
Vapor Density	No data available	(Air = 1.0)
Specific Gravity / Density	0,96	
Bulk Density	Not applicable	Liquid
Water Solubility	No information available	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Component	log Pow	
Ethanone, 1-[4-(2-methylpropyl)phenyl]-	3.4	
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
Viscosity	No data available	
Explosive Properties		explosive air/vapour mixtures possible
Oxidizing Properties	No information available	
Molecular Formula	C12 H16 O	
Molecular Weight	176.27	

SECTION 10. STABILITY AND REACTIVITY

Stability	Stable under normal conditions.
Hazardous Reactions	None under normal processing.
Hazardous Polymerization	Hazardous polymerization does not occur.
Conditions to Avoid	Incompatible products. Excess heat. Keep away from open flames, hot surfaces and sources of ignition.
Materials to avoid	Strong oxidizing agents. Strong bases. Reducing Agent.

Hazardous Decomposition Products Carbon monoxide (CO). Carbon dioxide (CO₂).

SECTION 11. TOXICOLOGICAL INFORMATION

Product Information

(a) acute toxicity;

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Ethanone, 1-[4-(2-methylpropyl)phenyl]-	LD50 = 5000 mg/kg (Rat)	>2000 mg/kg (Rabbit)	

(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	Category 1
	May cause sensitization by skin contact

(e) germ cell mutagenicity; No data available

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Not mutagenic in AMES Test

(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;

No data available

Target Organs

No information available.

(j) aspiration hazard;

No data available

Other Adverse Effects

The toxicological properties have not been fully investigated.

Symptoms / effects, both acute and delayed

Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting:
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

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	Microtox
Ethanone, 1-[4-(2-methylpropyl)phenyl]-	LC50: = 12.4 mg/L, 96h static (Lepomis macrochirus)	EC50: = 7.7 mg/L, 48h (Daphnia magna)		EC50 = 0.57 mg/L 5 min EC50 = 0.63 mg/L 15 min EC50 = 0.7 mg/L 30 min

Persistence and Degradability

Persistence

Not readily biodegradable

Degradation in sewage treatment plant

Persistence is unlikely.

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

Bioaccumulative Potential

Bioaccumulation is unlikely

Component	log Pow	Bioconcentration factor (BCF)
Ethanone, 1-[4-(2-methylpropyl)phenyl]-	3.4	No data available

Mobility in soil

No information available

Endocrine Disruptor Information

This product does not contain any known or suspected endocrine disruptors

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

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.

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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.

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**Road and Rail Transport**

UN-No UN1224
Proper Shipping Name Ketones, n.o.s
Technical Shipping Name Ethanone, 1-[4-(2-methylpropyl)phenyl]-
Hazard Class 3
Packing Group III

IMDG/IMO

UN-No UN1224
Proper Shipping Name Ketones, n.o.s
Technical Shipping Name Ethanone, 1-[4-(2-methylpropyl)phenyl]-
Hazard Class 3
Packing Group III

IATA

UN-No UN1224
Proper Shipping Name Ketones, n.o.s
Technical Shipping Name Ethanone, 1-[4-(2-methylpropyl)phenyl]-
Hazard Class 3
Packing Group III

Special Precautions for User No special precautions required

SECTION 15. REGULATORY INFORMATION**International Inventories**

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

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
Ethanone, 1-[4-(2-methylpropyl)phenyl]-	-	-	X	-	254-159-8	X	-	-	X	X	-	-

National Regulations

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SECTION 16. OTHER INFORMATION

Prepared By Health, Safety and Environmental Department
Creation Date 07-Jun-2012
Revision Date 26-Apr-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/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

PNEC - Predicted No Effect Concentration

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