

Material Safety Data Sheet

(1S,2S,3R,6S)-3-Acetoxy-3-methyl-6(1-methylethyl)-2(3-oxobutyl)cyclohexanenitrile, 99%

ACC# 71669

Section 1 - Chemical Product and Company Identification

Catalog Numbers: AC275190010

Synonyms: None.

Company Identification:

Acros Organics N.V.

One Reagent Lane

Fair Lawn, NJ 07410

For information in North America, call: 800-ACROS-01

For emergencies in the US, call CHEMTREC: 800-424-9300

Section 2 - Composition, Information on Ingredients

CAS#	Chemical Name	Percent	EINECS/ELINCS
131447-90-0	(1S,2S,3R,6S)-3-Acetoxy-3-methyl-6(1-methylethyl)-2(3-oxobutyl)cyclohexanenitrile	99	unlisted

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Appearance: slightly yellow crystalline powder.

Caution! May cause eye, skin, and respiratory tract irritation. Metabolized to cyanide in the body, which may cause headache, dizziness, weakness, unconsciousness, convulsions, coma and possible death. The toxicological properties of this material have not been fully investigated.

Target Organs: No data found.

Potential Health Effects

Eye: May cause eye irritation.

Skin: May cause skin irritation. May be metabolized to cyanide which in turn acts by inhibiting cytochrome oxidase impairing cellular respiration.

Ingestion: May cause irritation of the digestive tract. The toxicological properties of this substance have not been fully investigated. Metabolism may release cyanide, which may result in headache, dizziness, weakness, collapse, unconsciousness and possible death.

Inhalation: May cause respiratory tract irritation. The toxicological properties of this substance have not been fully investigated. May be metabolized to cyanide which in turn acts by inhibiting cytochrome oxidase impairing cellular respiration. Inhalation may result in symptoms similar to cyanide poisoning which include tachypnea, hyperpnea (abnormally rapid or deep breathing), and dyspnea (labored breathing) followed rapidly by respiratory depression. Pulmonary edema may occur.

Chronic: No information found. May be metabolized to cyanide which in turn acts by inhibiting cytochrome oxidase impairing cellular respiration. Chronic exposure to cyanide solutions may lead to the development of a "cyanide" rash, characterized by itching, and by macular, papular, and vesicular eruptions, and may be accompanied by secondary infections.

Section 4 - First Aid Measures

Eyes: Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical aid immediately.

Skin: Get medical aid. Flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse.

Ingestion: Never give anything by mouth to an unconscious person. Get medical aid immediately. Do NOT induce vomiting. If conscious and alert, rinse mouth and drink 2-4 cupfuls of milk or water.

Inhalation: Get medical aid immediately. Remove from exposure and move to fresh air immediately. If breathing is difficult, give oxygen. Do NOT use mouth-to-mouth resuscitation. If breathing has ceased apply artificial respiration using oxygen and a suitable mechanical device such as a bag and a mask.

Notes to Physician: May be partially metabolized to cyanide in the body.

Antidote: Always have a cyanide antidote kit on hand when working with cyanide compounds. Get medical advice to use.

Section 5 - Fire Fighting Measures

General Information: As in any fire, wear a self-contained breathing apparatus in pressure-demand, MSHA/NIOSH (approved or equivalent), and full protective gear. During a fire, irritating and highly toxic gases may be generated by thermal decomposition or combustion. Runoff from fire control or dilution water may cause pollution.

Extinguishing Media: Use agent most appropriate to extinguish fire. Use water spray, dry chemical, carbon dioxide, or appropriate foam.

Flash Point: Not applicable.

Autoignition Temperature: Not applicable.

Explosion Limits, Lower: Not available.

Upper: Not available.

NFPA Rating: (estimated) Health: 2; Flammability: 0; Instability: 0

Section 6 - Accidental Release Measures

General Information: Use proper personal protective equipment as indicated in Section 8.

Spills/Leaks: Vacuum or sweep up material and place into a suitable disposal container. Clean up spills immediately, observing precautions in the Protective Equipment section. Avoid generating dusty conditions. Provide ventilation.

Section 7 - Handling and Storage

Handling: Wash thoroughly after handling. Remove contaminated clothing and wash before reuse. Use with adequate ventilation. Minimize dust generation and accumulation. Avoid contact with eyes, skin, and clothing. Keep container tightly closed. Avoid ingestion and inhalation.

Storage: Keep container closed when not in use. Store in a tightly closed container. Keep refrigerated. (Store below 4°C/39°F.)

Section 8 - Exposure Controls, Personal Protection

Engineering Controls: Facilities storing or utilizing this material should be equipped with an eyewash facility and a safety shower. Use adequate ventilation to keep airborne concentrations low.

Exposure Limits

Chemical Name	ACGIH	NIOSH	OSHA - Final PELs
(1S,2S,3R,6S)-3-Acetoxy-3-methyl-6(1-methylethyl)-2(3-oxobutyl)cyclohexanenitrile	none listed	none listed	none listed

OSHA Vacated PELs: No OSHA Vacated PELs are listed for this chemical.

Personal Protective Equipment

Eyes: Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin: Wear appropriate protective gloves to prevent skin exposure.

Clothing: Wear appropriate protective clothing to prevent skin exposure.

Respirators: Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Section 9 - Physical and Chemical Properties

Physical State: Crystalline powder

Appearance: slightly yellow

Odor: Not available.

pH: Not available.

Vapor Pressure: Not available.

Vapor Density: Not available.

Evaporation Rate: Not available.

Viscosity: Not available.

Boiling Point: Not available.

Freezing/Melting Point: 106 - 109 deg C

Decomposition Temperature: Not available.

Solubility: practically insoluble

Specific Gravity/Density: Not available.

Molecular Formula: C₁₇H₂₇NO₃

Molecular Weight: 293.40

Section 10 - Stability and Reactivity

Chemical Stability: Stable under normal temperatures and pressures.

Conditions to Avoid: Incompatible materials, dust generation, excess heat, strong oxidants.

Incompatibilities with Other Materials: Oxidizing agents.

Hazardous Decomposition Products: Nitrogen oxides, carbon monoxide, irritating and toxic fumes and gases, carbon dioxide, nitrogen.

Hazardous Polymerization: Has not been reported

Section 11 - Toxicological Information

RTECS#:

CAS# 131447-90-0 unlisted.

LD50/LC50:

Not available.

Carcinogenicity:

CAS# 131447-90-0: Not listed by ACGIH, IARC, NTP, or CA Prop 65.

Epidemiology: No information found

Teratogenicity: No information found
Reproductive Effects: No information found
Mutagenicity: No information found
Neurotoxicity: No information found
Other Studies:

Section 12 - Ecological Information

No information available.

Section 13 - Disposal Considerations

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. US EPA guidelines for the classification determination are listed in 40 CFR Parts 261.3. Additionally, waste generators must consult state and local hazardous waste regulations to ensure complete and accurate classification.

RCRA P-Series: None listed.

RCRA U-Series: None listed.

Section 14 - Transport Information

	US DOT	Canada TDG
Shipping Name:	Not regulated as a hazardous material	No information available.
Hazard Class:		
UN Number:		
Packing Group:		

Section 15 - Regulatory Information

US FEDERAL

TSCA

CAS# 131447-90-0 is not listed on the TSCA inventory. It is for research and development use only.

Health & Safety Reporting List

None of the chemicals are on the Health & Safety Reporting List.

Chemical Test Rules

None of the chemicals in this product are under a Chemical Test Rule.

Section 12b

None of the chemicals are listed under TSCA Section 12b.

TSCA Significant New Use Rule

None of the chemicals in this material have a SNUR under TSCA.

CERCLA Hazardous Substances and corresponding RQs

None of the chemicals in this material have an RQ.

SARA Section 302 Extremely Hazardous Substances

None of the chemicals in this product have a TPQ.

Section 313

No chemicals are reportable under Section 313.

Clean Air Act:

This material does not contain any hazardous air pollutants.

This material does not contain any Class 1 Ozone depleters.

This material does not contain any Class 2 Ozone depleters.

Clean Water Act:

None of the chemicals in this product are listed as Hazardous Substances under the CWA.

None of the chemicals in this product are listed as Priority Pollutants under the CWA.

None of the chemicals in this product are listed as Toxic Pollutants under the CWA.

OSHA:

None of the chemicals in this product are considered highly hazardous by OSHA.

STATE

CAS# 131447-90-0 is not present on state lists from CA, PA, MN, MA, FL, or NJ.

California Prop 65

California No Significant Risk Level: None of the chemicals in this product are listed.

European/International Regulations

European Labeling in Accordance with EC Directives

Hazard Symbols:

XN

Risk Phrases:

R 20/21/22 Harmful by inhalation, in contact with skin and if swallowed.

Safety Phrases:

S 36/37 Wear suitable protective clothing and gloves.

WGK (Water Danger/Protection)

CAS# 131447-90-0: No information available.

Canada - DSL/NDSL

None of the chemicals in this product are listed on the DSL or NDSL list.

Canada - WHMIS

This product has a WHMIS classification of D2B.

This product has been classified in accordance with the hazard criteria of the Controlled Products Regulations and the MSDS contains all of the information required by those regulations.

Canadian Ingredient Disclosure List

Section 16 - Additional Information
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MSDS Creation Date: 9/02/1997

Revision #6 Date: 3/01/2006

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