

MATERIAL SAFETY DATA SHEET

Section No. 1 Identification of the substance and of the company/undertaking

1.1. Product Identifier:	3-Ketohexanoyl Coenzyme A, Free acid
SKU	A-84
CAS No.	19774-86-8
Index No.	N/A
EC No.	Not listed
EINECS No.	N/A
HS Code	UK: 2934 9990 90, USA: 2934 9990 01, Switzerland: 2934 9900, China: 2934 9990 99, Norway: 2934 9909, EU: 2934 9990
RTECS No.	N/A
REACH No.	Not registered
UFI No.	Not listed
1.2. Relevant identified uses of the substance or mixture and uses advised against	
Relevant identified uses	For research purposes only.
Uses advised against	Not for use by end consumers.
1.3. Details of the supplier of the safety data sheet	
Name	Essential Phosphates UAB
Address	Mokslininkų g. 12 LT-08412, Vilnius Lithuania
Telephone	+370 64729747
Email	info@coenzalabs.com
1.4. Emergency telephone number	
Manufacturers' phone	+370 64729747
Lithuanian toxicological information centre	+370 5 236 20528 +370 687 53 378

Section No. 2 Hazards Identification

2.1. Classification of the substance	Classification according to EU Regulation (EC) No 1272/2008 – not classified.
2.2. Label elements	Labelling according to Regulation (EC) No 1272/2008 – none.
Precautionary statement(s)	Not applicable.
2.3. Other hazards	The substance does not meet the criteria for PBT or vPvB substances in accordance with Annex XIII of Regulation (EC) No 1907/2006. The substance does not meet the criteria for substances identified under Article 59 as having endocrine disrupting properties in accordance with Regulation (EC) No 1907/2006.

Section No. 3 Composition / Information on Ingredients

3.1. Substances	
Component:	S-(2-(3-(4-((((5-(6-amino-9H-purin-9-yl)-4-hydroxy-3-(phosphonooxy)tetrahydrofuran-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)oxy)-2-hydroxy-3,3-dimethylbutanamido)propanamido)ethyl) 3-oxohexanethioate
EINECS No.	N/A
Reach No.	Not registered
Formula:	C ₂₇ H ₄₄ N ₇ O ₁₈ P ₃ S
Molecular Weight:	879.66 g/mol
CAS No.	19774-86-8

Purity:	≥ 95 %
Hazardous impurities	None
Stabilizers	None

Section No. 4 First Aid Measures

4.1. Description of first aid measure

General information:	Consult a physician. Show this safety data sheet to the doctor in attendance.
If inhaled:	Move person to fresh air. If not breathing, give artificial respiration. Consult a physician.
In case of skin contact:	Wash affected area with soap and water. Consult a physician if any exposure symptoms are observed.
In case of eye contact:	Immediately rinse eyes with plenty of water for at least 15 minutes. Consult a physician. Remove contact lenses. If eye irritation persists, consult a specialist.
If swallowed:	Rinse mouth with plenty of water. Do NOT induce vomiting unless advised to do so by a physician or Poison Control Centre.
Self-protection:	If needed protect yourself with FFP2 particle-filtering face mask. Take off contaminated clothes after first aid and take a shower with a plenty of water to fully remove contaminants.

4.2. Most important symptoms and effects, both acute and delayed

To the best of our knowledge, the chemical, physical and toxicological properties have not been thoroughly investigated. Possible effects may be:

Eye contact	Possible irritation, itching or redness.
Ingestion	Possible Irritation, nausea, vomiting.
Inhalation	Possible shortness of breath, coughing.
Skin contact	Possible irritation.

4.3. Indication of any immediate medical attention and special treatment needed

No data available. Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

Section No. 5 Fire and Explosion Data

5.1. Extinguishing media	Suitable extinguishing media: Carbon dioxide, foam, alcohol-resistant foam, dry chemical or water spray
5.2. Special hazards arising from the substance or mixture	Carbon oxides, nitrogen oxides, sulfur oxides, phosphorus oxides, in combustion may emit toxic fumes
5.3. Advice for firefighters	Wear self-contained breathing apparatus (according to EN 137) for firefighting if necessary and full-body protective clothing
5.4. Additional information	Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

Section No. 6 Accidental Release Measures

6.1. Personal precautions, protective equipment and emergency procedures

For non-emergency personnel

- Wear light protective suit, gloves and FFP2 particle filtering breathing mask.
- Avoid dust formation.
- Avoid breathing vapours, dust, mist or gas.
- Ensure adequate ventilation.
- Evacuate personnel to safe areas.

For emergency responders

- Protective equipment – wear respirator or breathing apparatus, protective suit, rubber boots and gloves as well as protective goggles.

6.2. Environmental precautions

Prevent further leakage or spillage of the substance. Take precautionary steps to avoid release of the substance into the environment.

6.3. Methods and materials for containment and cleaning up

Spilled product must be contained in suitable, closed containers for disposal (see Section 13). Disposal should be carried out in accordance with local applicable regulations. In case of large-scale product spillage inform the Fire Department and the Environmental Department of the Municipal Authority.

6.4. Reference to other sections

See section 7 for information on safe handling.

See section 8 for information on personal protection equipment.

See section 13 for information on disposal.

Section No. 7 Handling and Storage

7.1. Precautions for safe handling

- Avoid contact with eyes and skin.
- Avoid formation of dust and aerosols.
- Provide appropriate ventilation at places where dust is formed.
- Normal measures for preventive fire protection.
- Do not eat, drink or smoke in areas where the substance is being handled.
- After work with the substance wash your hands and other open skin areas with water and liquid soap.
- Contaminated clothes or other protective gowning must be taken off prior entering other areas, where product was not handled.

7.2. Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry, cool and well-ventilated area. Recommended storage temperature - 20°C.

The substance should be stored in areas protected from ignition source or open fire to prevent fire.

Recommendations for packaging: glass, polyethylene (PE), polypropylene (PP), polyamide (PA), polytetrafluoroethylene (PTFE).

Materials to be avoided: Substance must be protected from possible contact with strong basis and acids.

7.3. Specific end user(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

Section No. 8 Exposure Controls / Personal Protection

8.1. Control parameters

Contains no components with established occupational exposure limits.

8.2. Exposure control

Appropriate engineering controls

A laboratory fume hood or any other appropriate form of local exhaust ventilation shall be used to avoid exposure.

Personal protective equipment

For eye/face protection wear safety goggles or face shield. All used protective equipment should have been approved according to appropriate standards such as EN 166 (EU, CSA (Canada), NIOSH (US).

Skin/Body protection

- Handle with gloves.
- Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with the substance.
- Wear laboratory coat when handling small amounts of the substance. When working with the substance hood or adequate ventilation system is recommended.
- The selected protective gloves should satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.
- The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

- In a poorly ventilated area wear FFP2, FFP3 or NIOSH approved N100 particle filtering breathing mask.

- If the respirator is the sole means of protection, use a full-face supplied air respirator.

Environmental exposure controls

Avoid release of substance into the environment (air, drains, soil and water).

Section No. 9 Physical and Chemical Properties

9.1. Information on basic physical and chemical properties

Physical state:	Powder to crystalline powder
Colour:	White to slightly yellow
Odour:	Specific
pH:	No data available
Melting point/range:	No data available
Initial boiling point/range:	No data available
Boiling point:	No data available
Flash point:	No data available
Upper explosion limit:	No data available
Lower explosion limit:	No data available
Vapor pressure:	No data available
Water solubility:	Soluble
Other solubilities:	No data available
Partition coefficient (n-Octanol / Water):	No data available
Ignition temperature (n-Octanol / Water):	No data available
Decomposition temperature:	No data available
Viscosity:	No data available
Explosive properties:	Not classified as explosive
Oxidizing properties:	None

9.2. Other information

No data available

Section No. 10 Stability and Reactivity Data

10.1. Reactivity	Reacts with atmospheric oxygen.
10.2. Chemical stability	Stable under recommended storage conditions.
10.3. Possibility of hazardous reactions	No data available
10.4. Conditions to avoid	Air, moisture, heat.
10.5. Incompatible materials	Protect against strong acids and bases, as well as oxidising agents.
10.6. Hazardous decompositions products	Hazardous decomposition products formed under fire conditions. Nature of decomposition products not known.

Section No. 11 Toxicological Information

11.1. Information on toxicological effects

Acute toxicity	No data available
Skin corrosion/irritation	Based on practical experience substance does not cause corrosive or irritating effects on skin
Serious eye damage/irritation	The substance does not cause serious eye damage or irritation
Respiratory or skin sensitisation	Based on practical experience the substance does not cause sensitisation to the skin or the respiratory tract
Germ cell mutagenicity	No data available
Carcinogenicity	IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC. NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP. OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.
Reproductive toxicity	No data available

Specific target organ toxicity - single exposure	No data available
Specific target organ toxicity - repeated exposure	No data available
Aspiration hazard	No data available
Additional information	No data available

Section No. 12 Ecological Information

12.1. Toxicity	No data available
12.2. Persistence and degradability	No data available
12.3. Bio-accumulative potential	No data available
12.4. Mobility in soil	No data available
12.5. Results of PBT and vPvB assessment	Not applicable.
12.6. Results of endocrine-disrupting properties	Not applicable.
12.7. Other adverse effects	Discharge of material into the environment (water, soil etc.) must be avoided.

Section No. 13 Disposal Considerations

13.1 Waste treatment methods	
Product:	Do not discard unused product /substance into drainage system. Product/substance cannot be discarded along with municipal waste. Contact licensed professional waste disposal service Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.
Contaminated packaging:	Empty and well cleaned containers should be taken to an approved waste handling site for Recycling or disposal. Well cleaned containers may be submitted for recycling

Section No. 14 Transport Information

14.1. UN Number	ADN ADR/RID ICAO-TI / IATADGR IMDG	None None None None
14.2. UN Proper shipping name	ADN ADR/RID ICAO-TI / IATADGR IMDG	Not dangerous goods Not dangerous goods Not dangerous goods Not dangerous goods
14.3. Transport hazard class	ADN ADR/RID ICAO-TI / IATADGR IMDG	Not applicable Not applicable Not applicable Not applicable
14.4. Packaging group	ADN ADR/RID ICAO-TI / IATADGR IMDG	Not applicable Not applicable Not applicable Not applicable
14.5. Environmental hazards	ADN ADR/RID ICAO-TI / IATADGR IMDG	Not applicable Not applicable Not applicable Not applicable
14.6. Special precautions for user	Substance should be transported in well-enclosed containers, protected from the light and heat at the time of transportation. Temperature shall not exceed 25°C.	

14.7. Maritime transport in bulk Not applicable.
according to IMO
instruments

Section No. 15 Other Regulatory Information

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture
Regulation (EU) 649/2012 concerning the export and import of hazardous chemicals is not applicable

15.2. Chemical Safety Assessment

A Chemical Safety Assessment has not been required for this product.

Section No. 16 Other Information

16.1. Change Log

Version 1, 18 Feb, 2026

Original publication

16.2. Abbreviations and definitions

ADR	European Agreement concerning the International Carriage of Dangerous Goods by Road
CAS	Chemical Abstracts Service
EN	European Norm
EU	European Union
IATA-DGR	International Air Transport Association - Dangerous Goods Regulations
IBC Code	International Code for the Construction and Equipment of Ships Carrying Dangerous Chemicals
ICAO-TI	International Civil Aviation Organization - Technical Instructions
IMDG	International Maritime Code for Dangerous Goods
IMO	International Maritime Organisation
MARPOL	Maritime Pollution Convention
PBT	Persistent, Bio accumulative, and Toxic
REACH	Registration, Evaluation, and Authorisation of Chemicals
RID	Agreement on the Transport of Dangerous Goods by Rail
UFI	Unique Formulation Identifier
UN	United Nations, or: four-digit identification number of the substance or article taken from the
UN	Model Regulations
vPvB	very Persistent and very Bio accumulative

16.3. List of relevant R phrases, hazard statements, safety phrases and/or precautionary statements

None

16.4. Advice on any training

Employees, which are involved in any operations related to handling material, including manufacturing, packaging, handling or logistics should be familiar with the material safety data sheet.

16.5. Statement / Disclaimer

The purpose of information provided in the material safety data sheet is to ensure occupational health protection and safety, as well as environmental protection. All information provided in this material safety sheet to our best knowledge is believed to be accurate and representing current regulatory requirements. The above information was acquired by diligent search and the recommendations are based on prudent application of professional judgment. The information shall not be taken as being all inclusive and is to be used only as a guide. All materials and mixtures may present unknown hazards and should be used with caution. Since the Company cannot control the actual methods, volumes, or conditions of use, the Company shall not be held liable for any damages or losses resulting from the handling or from contact with the product as described herein.