



Ecgonine Methyl Ester-D3

Novachem Pty Ltd

Version No: 3.4

Safety Data Sheet according to WHS Regulations (Hazardous Chemicals) Amendment 2020 and ADG requirements

Chemwatch Hazard Alert Code: 4

Issue Date: 07/07/2023

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S.GHS.AUS.EN

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

Product Identifier

Product name	Ecgonine Methyl Ester-D3
Chemical Name	ecgonine methyl ester-D3
Synonyms	E-002
Proper shipping name	ACETONITRILE
Other means of identification	E-002
CAS number	136765-34-9*

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

Relevant identified uses	Laboratory certified chemical reference material
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Details of the manufacturer or supplier of the safety data sheet

Registered company name	Novachem Pty Ltd	Novachem Pty Ltd
Address	25 Crissane Road, Heidelberg West Victoria 3081 Australia	25 Crissane Road, Heidelberg West Victoria 3081 Australia
Telephone	+61384151255	+61384151255
Fax	+61386250088	+61386250088
Website	www.novachem.com.au	www.novachem.com.au
Email	novachem@novachem.com.au	novachem@novachem.com.au

Emergency telephone number

Association / Organisation	Victorian Poisons Information Centre	Victorian Poisons Information Centre
Emergency telephone numbers	13 11 26	13 11 26
Other emergency telephone numbers	Not Available	Not Available

SECTION 2 Hazards identification

Classification of the substance or mixture

Poisons Schedule	S9
Classification [1]	Flammable Liquids Category 2, Acute Toxicity (Oral) Category 4, Acute Toxicity (Dermal) Category 4, Serious Eye Damage/Eye Irritation Category 2A, Acute Toxicity (Inhalation) Category 4
Legend:	1. Classified by Chemwatch; 2. Classification drawn from HCIS; 3. Classification drawn from Regulation (EU) No 1272/2008 - Annex VI

Label elements

Hazard pictogram(s)	
Signal word	Danger

Hazard statement(s)

H225	Highly flammable liquid and vapour.
H302	Harmful if swallowed.
H312	Harmful in contact with skin.

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H319	Causes serious eye irritation.
H332	Harmful if inhaled.

Precautionary statement(s) Prevention

P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233	Keep container tightly closed.
P271	Use only outdoors or in a well-ventilated area.
P240	Ground and bond container and receiving equipment.

Precautionary statement(s) Response

P370+P378	In case of fire: Use alcohol resistant foam or fine spray/water fog to extinguish.
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.
P301+P312	IF SWALLOWED: Call a POISON CENTER/doctor/physician/first aider if you feel unwell.

Precautionary statement(s) Storage

P403+P235	Store in a well-ventilated place. Keep cool.
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Precautionary statement(s) Disposal

P501	Dispose of contents/container to authorised hazardous or special waste collection point in accordance with any local regulation.
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SECTION 3 Composition / information on ingredients

Substances

CAS No	%[weight]	Name
75-05-8	99.99	acetonitrile
136765-34-9*	0.01	Ecgonine Methyl Ester-D3

Legend: 1. Classified by Chemwatch; 2. Classification drawn from HCIS; 3. Classification drawn from Regulation (EU) No 1272/2008 - Annex VI; 4. Classification drawn from C&L; * EU IOELVs available

Mixtures

See section above for composition of Substances

SECTION 4 First aid measures

Description of first aid measures

Eye Contact	<p>If this product comes in contact with the eyes:</p> <ul style="list-style-type: none"> ▶ Immediately hold eyelids apart and flush the eye continuously with running water. ▶ Ensure complete irrigation of the eye by keeping eyelids apart and away from eye and moving the eyelids by occasionally lifting the upper and lower lids. ▶ Continue flushing until advised to stop by the Poisons Information Centre or a doctor, or for at least 15 minutes. ▶ Transport to hospital or doctor without delay. ▶ Removal of contact lenses after an eye injury should only be undertaken by skilled personnel.
Skin Contact	<p>If skin or hair contact occurs:</p> <ul style="list-style-type: none"> ▶ Quickly but gently, wipe material off skin with a dry, clean cloth. ▶ Immediately remove all contaminated clothing, including footwear. ▶ Wash skin and hair with running water. Continue flushing with water until advised to stop by the Poisons Information Centre. ▶ Transport to hospital, or doctor.
Inhalation	<ul style="list-style-type: none"> ▶ If fumes or combustion products are inhaled remove from contaminated area. ▶ Lay patient down. Keep warm and rested. ▶ Prostheses such as false teeth, which may block airway, should be removed, where possible, prior to initiating first aid procedures. ▶ Apply artificial respiration if not breathing, preferably with a demand valve resuscitator, bag-valve mask device, or pocket mask as trained. Perform CPR if necessary. ▶ Transport to hospital, or doctor, without delay.
Ingestion	<ul style="list-style-type: none"> ▶ IF SWALLOWED, REFER FOR MEDICAL ATTENTION, WHERE POSSIBLE, WITHOUT DELAY. ▶ For advice, contact a Poisons Information Centre or a doctor. ▶ Urgent hospital treatment is likely to be needed. ▶ In the mean time, qualified first-aid personnel should treat the patient following observation and employing supportive measures as indicated by the patient's condition. ▶ If the services of a medical officer or medical doctor are readily available, the patient should be placed in his/her care and a copy of the SDS should be provided. Further action will be the responsibility of the medical specialist. ▶ If medical attention is not available on the worksite or surroundings send the patient to a hospital together with a copy of the SDS. <p>Where medical attention is not immediately available or where the patient is more than 15 minutes from a hospital or unless instructed otherwise:</p> <ul style="list-style-type: none"> ▶ INDUCE vomiting with fingers down the back of the throat, ONLY IF CONSCIOUS. Lean patient forward or place on left side (head-down position, if possible) to maintain open airway and prevent aspiration. <p>NOTE: Wear a protective glove when inducing vomiting by mechanical means.</p>

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Indication of any immediate medical attention and special treatment needed

For cyanide intoxication (and for certain nitriles which produce cyanide ion)

- ▶ Signs symptoms of acute cyanide poisoning reflect cellular hypoxia and are often non-specific.
- ▶ Cyanosis may be a late finding.
- ▶ A *bradycardic*, hypertensive and tachypneic patient suggests poisoning especially if CNS and cardiovascular depression subsequently occurs.
- ▶ Immediate attention should be directed towards assisted ventilation, administration of 100% oxygen, insertion of intravenous lines and institution of cardiac monitoring.
- ▶ Obtain an arterial blood gas immediately and correct any severe metabolic acidosis (pH below 7.15).
- ▶ Mildly symptomatic patients generally require supportive care alone. Nitrites should not be given indiscriminately - in all cases of moderate to severe poisoning, they should be given in conjunction with thiosulfate. As a temporizing measure supply amyl nitrite perles (0.2ml inhaled 30 seconds every minute) until intravenous lines for sodium nitrite are established. 10 ml of a 3% solution is administered over 4 minutes to produce 20% methaemoglobin in adults. Follow directly with 50 ml of 25% sodium thiosulfate, at the same rate, IV. If symptoms reappear or persist within 1/2-1 hour, repeat nitrite and thiosulfate at 50% of initial dose. As the mode of action involves the metabolic conversion of the thiosulfate to thiocyanate, renal failure may enhance thiocyanate toxicity.
- ▶ Methylene blue is not an antidote. [Ellenhorn and Barceloux: Medical Toxicology]

If amyl nitrite intervention is employed then Medical Treatment Kits should contain the following:

- ▶ One box containing one dozen amyl nitrite ampoules
- ▶ Two sterile ampoules of sodium nitrite solution (10 mL of a 3% solution in each)
- ▶ Two sterile ampoules of sodium thiosulfate solution (50 mL of a 25% solution in each)
- ▶ One 10 mL sterile syringe. One 50 mL sterile syringe. Two sterile intravenous needles. One tourniquet.
- ▶ One dozen gauze pads.
- ▶ Latex gloves
- ▶ A "Biohazard" bag for disposal of bloody/contaminated equipment.
- ▶ A set of cyanide instructions on first aid and medical treatment.

- Notes on the use of amyl nitrite:-

- ▶ AN is highly volatile and flammable - do not smoke or use around a source of ignition.
- ▶ If treating patient in a windy or draughty area provide some shelter or protection (shirt, wall, drum, cupped hand etc.) to prevent amyl nitrite vapour from being blown away. Keep ampoule upwind from the nose, the objective is to get amyl nitrite into the patients lungs.
- ▶ Rescuers should avoid AN inhalation to avoid becoming dizzy and losing competence.
- ▶ Lay the patient down. Since AN dilates blood vessels and lowers blood pressure, lying down will help keep patient conscious.
- ▶ **DO NOT overuse - excessive use might put the patient into shock.** Experience at DuPont plants has not shown any serious after-effects from treatment with amyl nitrite.

ADDITIONAL NOTES:

- ▶ Major medical treatment procedures may vary e.g. US (FDA method as recommended by DuPont) uses amyl nitrite as a methaemoglobin generator, followed by treatment with sodium nitrite and then sodium thiosulfate.

MODES OF ACTION: Amyl nitrite (AN) reacts with haemoglobin (HB) to form about 5% methaemoglobin (MHB). Sodium nitrite (NaNO₂) reacts with haemoglobin to form approximately 20-30% methaemoglobin. Methaemoglobin attracts cyanide ions (CN) from tissue and binds with them to become cyanmethaemoglobin (CNMHB). Sodium thiosulfate (Na₂S₂O₃) converts cyanmethaemoglobin to thiocyanate (HSCN) which is excreted by the kidneys. i.e. AN + HB = MHB NaNO₂ + HB = MHB CN + MHB = CNMHB Na₂S₂O₃ + CNMHB + O₂ = HSCN

- ▶ The administration of the antidote salts is intravenous in normal saline, Ringers lactate or other available IV fluid.
- ▶ European practice may use 4-dimethylaminophenol (DMAP) as a methaemoglobin generator. Also hydroxycobalamin (Vitamin B12a) is used. Hydroxycobalamin works by reacting with cyanide to form cyanocobalamin (Vitamin B12) which is excreted in the urine.
- ▶ European and Australian NOHSC (ASCC) propose dicobalt edetate (Kelocyanor) as antidote. This acts by chelating cyanide to form stable cobaltcyanide, which is excreted in the urine. In all cases hyperbaric therapy may increase the efficiency of a cyanide antidote kit.

SECTION 5 Firefighting measures

Extinguishing media

- ▶ Foam.
- ▶ Dry chemical powder.
- ▶ BCF (where regulations permit).
- ▶ Carbon dioxide.

Special hazards arising from the substrate or mixture

Fire Incompatibility	▶ Avoid contamination with oxidising agents i.e. nitrates, oxidising acids, chlorine bleaches, pool chlorine etc. as ignition may result
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Advice for firefighters

Fire Fighting	<ul style="list-style-type: none"> ▶ Alert Fire Brigade and tell them location and nature of hazard. ▶ May be violently or explosively reactive. ▶ Wear full body protective clothing with breathing apparatus. ▶ Prevent, by any means available, spillage from entering drains or water course.
Fire/Explosion Hazard	Combustion products include: carbon dioxide (CO ₂) <ul style="list-style-type: none"> ▶ Liquid and vapour are highly flammable. ▶ Severe fire hazard when exposed to heat, flame and/or oxidisers. ▶ Vapour forms an explosive mixture with air. ▶ Severe explosion hazard, in the form of vapour, when exposed to flame or spark. nitrogen oxides (NO _x) other pyrolysis products typical of burning organic material.
HAZCHEM	•2YE

SECTION 6 Accidental release measures

Personal precautions, protective equipment and emergency procedures

See section 8

Environmental precautions

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See section 12

Methods and material for containment and cleaning up

Minor Spills	<p>Environmental hazard - contain spillage.</p> <ul style="list-style-type: none"> ▶ Remove all ignition sources. ▶ Clean up all spills immediately. ▶ Avoid breathing vapours and contact with skin and eyes. ▶ Control personal contact with the substance, by using protective equipment.
Major Spills	<p>Environmental hazard - contain spillage.</p> <ul style="list-style-type: none"> ▶ DO NOT touch the spill material <p>For alkyl nitriles: For residue:</p> <ul style="list-style-type: none"> ▶ Add alkaline hypochlorite solution to spill to produce cyanate. ▶ Neutralise liquid, and absorb with sawdust. ▶ Collect solid residues and seal in drums for disposal. ▶ Wash spill area with large quantities of water. ▶ Clear area of personnel and move upwind. ▶ Alert Fire Brigade and tell them location and nature of hazard. ▶ May be violently or explosively reactive. ▶ Wear full body protective clothing with breathing apparatus.

Personal Protective Equipment advice is contained in Section 8 of the SDS.

SECTION 7 Handling and storage

Precautions for safe handling

Safe handling	<ul style="list-style-type: none"> ▶ Containers, even those that have been emptied, may contain explosive vapours. ▶ Do NOT cut, drill, grind, weld or perform similar operations on or near containers. ▶ Avoid all personal contact, including inhalation. ▶ Wear protective clothing when risk of exposure occurs. ▶ Use in a well-ventilated area. ▶ Prevent concentration in hollows and sumps.
Other information	<ul style="list-style-type: none"> ▶ Store in original containers in approved flame-proof area. ▶ No smoking, naked lights, heat or ignition sources. ▶ DO NOT store in pits, depression, basement or areas where vapours may be trapped. ▶ Keep containers securely sealed.

Conditions for safe storage, including any incompatibilities

Suitable container	<ul style="list-style-type: none"> ▶ Glass container is suitable for laboratory quantities ▶ Packing as supplied by manufacturer. ▶ Plastic containers may only be used if approved for flammable liquid. ▶ Check that containers are clearly labelled and free from leaks. ▶ For low viscosity materials (i) : Drums and jerry cans must be of the non-removable head type. (ii) : Where a can is to be used as an inner package, the can must have a screwed enclosure. ▶ For materials with a viscosity of at least 2680 cSt. (23 deg. C) ▶ For manufactured product having a viscosity of at least 250 cSt.
Storage incompatibility	<p>Acetonitrile</p> <ul style="list-style-type: none"> ▶ forms cyanide gas on contact with steam ▶ reacts violently with oxidisers such as chlorine, bromine, fluorine; with chlorosulfonic acid, oleum or sulfuric acid ▶ is incompatible with water (especially if acid or alkaline), acids, caustics, nitrating agents, indium, nitrogen tetroxide , sulfur trioxide, iron(III) salts of perchlorate, nitrogen fluoride compounds ▶ attacks most rubber and plastics ▶ may accumulate electrical charges, causing ignition of vapours ▶ Contact with acids produces toxic fumes ▶ Nitriles may polymerise in the presence of metals and some metal compounds. ▶ They are incompatible with acids; mixing nitriles with strong oxidising acids can lead to extremely violent reactions. ▶ Nitriles are generally incompatible with other oxidising agents such as peroxides and epoxides. ▶ The combination of bases and nitriles can produce hydrogen cyanide. ▶ The covalent cyano group is endothermic and many organic nitriles are reactive under certain conditions; N-cyano derivatives are reactive or unstable. ▶ The majority of endothermic compounds are thermodynamically unstable and may decompose explosively under various circumstances of initiation. ▶ Many but not all endothermic compounds have been involved in decompositions, reactions and explosions and, in general, compounds with significantly positive values of standard heats of formation, may be considered suspect on stability grounds. <p>BREThERICK L.: Handbook of Reactive Chemical Hazards</p> <p>WARNING:</p> <p>May decompose violently or explosively on contact with other substances.</p> <ul style="list-style-type: none"> ▶ This substance, or one of its components, is one of the relatively few compounds which are described as "endothermic" i.e. heat is absorbed into the compound, rather than released from it, during its formation. ▶ The majority of endothermic compounds are thermodynamically unstable and may decompose explosively under various circumstances of initiation. ▶ Many but not all endothermic compounds have been involved in decompositions, reactions and explosions and, in general, compounds with significantly positive values of standard heats of formation, may be considered suspect on stability grounds. ▶ Avoid reaction with oxidising agents

SECTION 8 Exposure controls / personal protection

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Control parameters

Occupational Exposure Limits (OEL)

INGREDIENT DATA

Source	Ingredient	Material name	TWA	STEL	Peak	Notes
Australia Exposure Standards	acetonitrile	Acetonitrile	40 ppm / 67 mg/m3	101 mg/m3 / 60 ppm	Not Available	Not Available

Emergency Limits

Ingredient	TEEL-1	TEEL-2	TEEL-3
acetonitrile	Not Available	Not Available	Not Available


Ingredient	Original IDLH	Revised IDLH
acetonitrile	500 ppm	137 ppm
Ecgonine Methyl Ester-D3	Not Available	Not Available

Occupational Exposure Banding

Ingredient	Occupational Exposure Band Rating	Occupational Exposure Band Limit
Ecgonine Methyl Ester-D3	E	≤ 0.1 ppm

Notes: Occupational exposure banding is a process of assigning chemicals into specific categories or bands based on a chemical's potency and the adverse health outcomes associated with exposure. The output of this process is an occupational exposure band (OEB), which corresponds to a range of exposure concentrations that are expected to protect worker health.

Exposure controls

Appropriate engineering controls	<p>Engineering controls are used to remove a hazard or place a barrier between the worker and the hazard. Well-designed engineering controls can be highly effective in protecting workers and will typically be independent of worker interactions to provide this high level of protection.</p> <p>The basic types of engineering controls are:</p> <ul style="list-style-type: none"> Process controls which involve changing the way a job activity or process is done to reduce the risk. Enclosure and/or isolation of emission source which keeps a selected hazard "physically" away from the worker and ventilation that strategically "adds" and "removes" air in the work environment.
Individual protection measures, such as personal protective equipment	
Eye and face protection	<ul style="list-style-type: none"> Safety glasses with side shields. Chemical goggles. [AS/NZS 1337.1, EN166 or national equivalent] Contact lenses may pose a special hazard; soft contact lenses may absorb and concentrate irritants. A written policy document, describing the wearing of lenses or restrictions on use, should be created for each workplace or task.
Skin protection	See Hand protection below
Hands/feet protection	<ul style="list-style-type: none"> Wear chemical protective gloves, e.g. PVC. Wear safety footwear or safety gumboots, e.g. Rubber <p>The selection of suitable gloves does not only depend on the material, but also on further marks of quality which vary from manufacturer to manufacturer. Where the chemical is a preparation of several substances, the resistance of the glove material can not be calculated in advance and has therefore to be checked prior to the application.</p> <p>The exact break through time for substances has to be obtained from the manufacturer of the protective gloves and has to be observed when making a final choice.</p> <p>Personal hygiene is a key element of effective hand care.</p> <p>for acetonitrile: Butyl rubber, PVAL, Teflon, Saranex, Silvershield, Viton/ chlorobutyl are all highly resistant to permeation</p>
Body protection	See Other protection below
Other protection	<ul style="list-style-type: none"> Overalls. PVC Apron. PVC protective suit may be required if exposure severe. Eyewash unit. Some plastic personal protective equipment (PPE) (e.g. gloves, aprons, overshoes) are not recommended as they may produce static electricity. For large scale or continuous use wear tight-weave non-static clothing (no metallic fasteners, cuffs or pockets). Non sparking safety or conductive footwear should be considered. Conductive footwear describes a boot or shoe with a sole made from a conductive compound chemically bound to the bottom components, for permanent control to electrically ground the foot an shall dissipate static electricity from the body to reduce the possibility of ignition of volatile compounds.

Recommended material(s)

GLOVE SELECTION INDEX

Glove selection is based on a modified presentation of the:

"Forsberg Clothing Performance Index".

The effect(s) of the following substance(s) are taken into account in the **computer-generated** selection:

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Material	CPI
BUTYL	A
BUTYL/NEOPRENE	A

Respiratory protection

Type A Filter of sufficient capacity. (AS/NZS 1716 & 1715, EN 143:2000 & 149:2001, ANSI Z88 or national equivalent)

Selection of the Class and Type of respirator will depend upon the level of breathing zone contaminant and the chemical nature of the contaminant. Protection Factors (defined as the ratio of contaminant outside and inside the mask) may also be important.

Required minimum protection factor	Maximum gas/vapour concentration present in air p.p.m. (by volume)	Half-face Respirator	Full-Face Respirator
up to 10	1000	A-AUS / Class1	-

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CPE	A
PE/EVAL/PE	A
PVA	A
SARANEX-23	A
NEOPRENE	B
TEFLON	B
NATURAL RUBBER	C
NATURAL+NEOPRENE	C
NITRILE	C
VITON/NEOPRENE	C

* CPI - Chemwatch Performance Index

A: Best Selection

B: Satisfactory; may degrade after 4 hours continuous immersion

C: Poor to Dangerous Choice for other than short term immersion

NOTE: As a series of factors will influence the actual performance of the glove, a final selection must be based on detailed observation. -

* Where the glove is to be used on a short term, casual or infrequent basis, factors such as "feel" or convenience (e.g. disposability), may dictate a choice of gloves which might otherwise be unsuitable following long-term or frequent use. A qualified practitioner should be consulted.

up to 50	1000	-	A-AUS / Class 1
up to 50	5000	Airline *	-
up to 100	5000	-	A-2
up to 100	10000	-	A-3
100+			Airline**

* - Continuous Flow ** - Continuous-flow or positive pressure demand

A(All classes) = Organic vapours, B AUS or B1 = Acid gasses, B2 = Acid gas or hydrogen cyanide(HCN), B3 = Acid gas or hydrogen cyanide(HCN), E = Sulfur dioxide(SO2), G = Agricultural chemicals, K = Ammonia(NH3), Hg = Mercury, NO = Oxides of nitrogen, MB = Methyl bromide, AX = Low boiling point organic compounds(below 65 degC)

- ▶ Cartridge respirators should never be used for emergency ingress or in areas of unknown vapour concentrations or oxygen content.
- ▶ The wearer must be warned to leave the contaminated area immediately on detecting any odours through the respirator. The odour may indicate that the mask is not functioning properly, that the vapour concentration is too high, or that the mask is not properly fitted. Because of these limitations, only restricted use of cartridge respirators is considered appropriate.
- ▶ Cartridge performance is affected by humidity. Cartridges should be changed after 2 hr of continuous use unless it is determined that the humidity is less than 75%, in which case, cartridges can be used for 4 hr. Used cartridges should be discarded daily, regardless of the length of time used

SECTION 9 Physical and chemical properties

Information on basic physical and chemical properties

Appearance	Not Available		
Physical state	Liquid	Relative density (Water = 1)	0.8
Odour	Not Available	Partition coefficient n-octanol / water	Not Available
Odour threshold	Not Available	Auto-ignition temperature (°C)	524.0
pH (as supplied)	Not Applicable	Decomposition temperature (°C)	Not Available
Melting point / freezing point (°C)	-45	Viscosity (cSt)	Not Available
Initial boiling point and boiling range (°C)	81.1	Molecular weight (g/mol)	41.05 Pure
Flash point (°C)	5.5 (OC)	Taste	Not Available
Evaporation rate	5.79 BuAc=1 BuAC = 1	Explosive properties	Not Available
Flammability	HIGHLY FLAMMABLE.	Oxidising properties	Not Available
Upper Explosive Limit (%)	16.0	Surface Tension (dyn/cm or mN/m)	Not Available
Lower Explosive Limit (%)	4.4	Volatile Component (%vol)	100
Vapour pressure (kPa)	13.3 @ 27 deg.C	Gas group	Not Available
Solubility in water	Miscible	pH as a solution (1%)	Not Available
Vapour density (Air = 1)	1.4	VOC g/L	Not Available

SECTION 10 Stability and reactivity

Reactivity	See section 7
Chemical stability	<ul style="list-style-type: none"> ▶ Presence of elevated temperatures. ▶ Unstable in the presence of incompatible materials. ▶ Product is considered stable. ▶ Hazardous polymerisation will not occur.
Possibility of hazardous reactions	See section 7
Conditions to avoid	See section 7
Incompatible materials	See section 7
Hazardous decomposition products	See section 5

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SECTION 11 Toxicological information

Information on toxicological effects

Inhaled	Inhalation of vapours or aerosols (mists, fumes), generated by the material during the course of normal handling, may produce toxic effects. The material is not thought to produce respiratory irritation (as classified by EC Directives using animal models). Nevertheless inhalation of vapours, fumes or aerosols, especially for prolonged periods, may produce respiratory discomfort and occasionally, distress. There is strong evidence to suggest that this material can cause, if inhaled once, serious, irreversible damage of organs. The smell of acetonitrile does not give enough warning of exposure. The gas is highly toxic, and inhaling it can cause loss of consciousness.
Ingestion	Severely toxic effects may result from the accidental ingestion of the material; animal experiments indicate that ingestion of less than 5 gram may be fatal or may produce serious damage to the health of the individual. Strong evidence exists that exposure to the material may cause irreversible damage (other than cancer, mutations and birth defects) following a single exposure by swallowing. Nitrile poisoning exhibits similar symptoms to poisoning due to hydrogen cyanide. The substances irritate the eyes and skin, and are absorbed quickly and completely through the skin. Cyanide poisoning can cause increased saliva output, nausea without vomiting, anxiety, confusion, vertigo, dizziness, stiffness of the lower jaw, convulsions, spasm, paralysis, coma and irregular heartbeat, and stimulation of breathing followed by failure. Often the skin becomes cyanosed (blue-grey), and this is often delayed.
Skin Contact	There is strong evidence to suggest that this material, on a single contact with skin, can cause serious, irreversible damage of organs. The material is not thought to be a skin irritant (as classified by EC Directives using animal models). Temporary discomfort, however, may result from prolonged dermal exposures. Open cuts, abraded or irritated skin should not be exposed to this material. Entry into the blood-stream, through, for example, cuts, abrasions or lesions, may produce systemic injury with harmful effects. Examine the skin prior to the use of the material and ensure that any external damage is suitably protected. Skin contact with the material may produce toxic effects; systemic effects may result following absorption.
Eye	There is evidence that material may produce eye irritation in some persons and produce eye damage 24 hours or more after instillation. Severe inflammation may be expected with pain.
Chronic	Repeated or long-term occupational exposure is likely to produce cumulative health effects involving organs or biochemical systems. Chronic exposure to cyanides and certain nitriles may result in interference to iodine uptake by thyroid gland and its consequent enlargement. This occurs following metabolic conversion of the cyanide moiety to thiocyanate.

Ecgonine Methyl Ester-D3	TOXICITY	IRRITATION
	Not Available	Not Available
acetonitrile	TOXICITY	IRRITATION
	Dermal (rabbit) LD50: >2000 mg/kg ^[1]	Eye (rabbit):20 mg (open)-SEVERE
	Inhalation(Rabbit) LC50; 2828 ppm4h ^[2]	Skin (rabbit):500 mg (open)-mild
	Oral (Rabbit) LD50; 50 mg/kg ^[2]	
Legend:	1. Value obtained from Europe ECHA Registered Substances - Acute toxicity 2. Value obtained from manufacturer's SDS. Unless otherwise specified data extracted from RTECS - Register of Toxic Effect of chemical Substances	

ACETONITRILE	The material may produce severe irritation to the eye causing pronounced inflammation. Repeated or prolonged exposure to irritants may produce conjunctivitis. The material may cause skin irritation after prolonged or repeated exposure and may produce on contact skin redness, swelling, the production of vesicles, scaling and thickening of the skin.
Ecgonine Methyl Ester-D3 & ACETONITRILE	Absorption of acetonitrile occurs after oral, skin, or inhalation exposure. The liquid or vapour is irritating to the skin, eyes, and airways. At high enough doses, death can occur quickly from respiratory failure. Lower doses cause typical symptoms of cyanide poisoning such as salivation, nausea, vomiting, anxiety, confusion, rapid and difficult breathing, rapid pulse, unconsciousness, and convulsions.

Acute Toxicity	✓	Carcinogenicity	✗
Skin Irritation/Corrosion	✗	Reproductivity	✗
Serious Eye Damage/Irritation	✓	STOT - Single Exposure	✗
Respiratory or Skin sensitisation	✗	STOT - Repeated Exposure	✗
Mutagenicity	✗	Aspiration Hazard	✗

Legend: ✗ – Data either not available or does not fill the criteria for classification
 ✓ – Data available to make classification

SECTION 12 Ecological information

Toxicity

Ecgonine Methyl Ester-D3	Endpoint	Test Duration (hr)	Species	Value	Source
	Not Available	Not Available	Not Available	Not Available	Not Available
acetonitrile	Endpoint	Test Duration (hr)	Species	Value	Source
	EC50	72h	Algae or other aquatic plants	>1000mg/l	2
	EC50	48h	Crustacea	>1000mg/l	2

Continued...

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LC50	96h	Fish	>100mg/l	2
NOEC(ECx)	24h	Crustacea	0.00001mg/l	4

Legend: Extracted from 1. IUCLID Toxicity Data 2. Europe ECHA Registered Substances - Ecotoxicological Information - Aquatic Toxicity 4. US EPA, Ecotox database - Aquatic Toxicity Data 5. ECETOC Aquatic Hazard Assessment Data 6. NITE (Japan) - Bioconcentration Data 7. METI (Japan) - Bioconcentration Data 8. Vendor Data

On the basis of available evidence concerning either toxicity, persistence, potential to accumulate and/or observed environmental fate and behaviour, the material may present a danger, immediate or long-term and/or delayed, to the structure and/or functioning of natural ecosystems.

Soil Guidelines: Dutch Criteria:

free cyanide: 1 mg/kg (target)

20 mg/kg (intervention)

complex cyanide (pH 5): 5 mg/kg (target)

50 mg/kg (intervention)

Air Quality Standards: no safe guidelines recommended due to carcinogenic properties.

DO NOT discharge into sewer or waterways.

Abiotic Effects: Acetonitrile is a volatile organic compound (VOC) substance, thus it is a contributor to the formation of photochemical smog in the presence of other VOCs.

Transport: Acetonitrile is primarily removed by volatilization and leaching into groundwater. It has low adsorption potential to soils. Air - Acetonitrile may persist in the troposphere and can be transported over long distances.

Persistence and degradability

Ingredient	Persistence: Water/Soil	Persistence: Air
acetonitrile	HIGH (Half-life = 360 days)	HIGH (Half-life = 541.29 days)

Bioaccumulative potential

Ingredient	Bioaccumulation
acetonitrile	LOW (BCF = 0.4)

Mobility in soil

Ingredient	Mobility
acetonitrile	LOW (KOC = 4.5)

SECTION 13 Disposal considerations

Waste treatment methods

Product / Packaging disposal	<ul style="list-style-type: none"> ▶ Containers may still present a chemical hazard/ danger when empty. ▶ Return to supplier for reuse/ recycling if possible. <p>Otherwise:</p> <ul style="list-style-type: none"> ▶ If container can not be cleaned sufficiently well to ensure that residuals do not remain or if the container cannot be used to store the same product, then puncture containers, to prevent re-use, and bury at an authorised landfill. ▶ Where possible retain label warnings and SDS and observe all notices pertaining to the product. <p>Legislation addressing waste disposal requirements may differ by country, state and/ or territory. Each user must refer to laws operating in their area. In some areas, certain wastes must be tracked.</p> <p>A Hierarchy of Controls seems to be common - the user should investigate:</p> <ul style="list-style-type: none"> ▶ Reduction ▶ Reuse ▶ Recycling ▶ Disposal (if all else fails) <p>This material may be recycled if unused, or if it has not been contaminated so as to make it unsuitable for its intended use.</p> <ul style="list-style-type: none"> ▶ DO NOT allow wash water from cleaning or process equipment to enter drains. ▶ It may be necessary to collect all wash water for treatment before disposal. ▶ In all cases disposal to sewer may be subject to local laws and regulations and these should be considered first. ▶ Where in doubt contact the responsible authority. ▶ Recycle wherever possible. ▶ Consult manufacturer for recycling options or consult local or regional waste management authority for disposal if no suitable treatment or disposal facility can be identified. ▶ Dispose of by: burial in a land-fill specifically licensed to accept chemical and / or pharmaceutical wastes or Incineration in a licensed apparatus (after admixture with suitable combustible material). ▶ Decontaminate empty containers.
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SECTION 14 Transport information

Labels Required

	
Marine Pollutant	NO
HAZCHEM	*2YE

Land transport (ADG)

UN number or ID number	1648
UN proper shipping name	ACETONITRILE

Ecgonine Methyl Ester-D3

Transport hazard class(es)	Class	3
	Subsidiary risk	Not Applicable
Packing group	II	
Environmental hazard	Not Applicable	
Special precautions for user	Special provisions	Not Applicable
	Limited quantity	1 L

Air transport (ICAO-IATA / DGR)

UN number	1648	
UN proper shipping name	Acetonitrile	
Transport hazard class(es)	ICAO/IATA Class	3
	ICAO / IATA Subrisk	Not Applicable
	ERG Code	3L
Packing group	II	
Environmental hazard	Not Applicable	
Special precautions for user	Special provisions	Not Applicable
	Cargo Only Packing Instructions	364
	Cargo Only Maximum Qty / Pack	60 L
	Passenger and Cargo Packing Instructions	353
	Passenger and Cargo Maximum Qty / Pack	5 L
	Passenger and Cargo Limited Quantity Packing Instructions	Y341
	Passenger and Cargo Limited Maximum Qty / Pack	1 L

Sea transport (IMDG-Code / GGVSee)

UN number	1648	
UN proper shipping name	ACETONITRILE	
Transport hazard class(es)	IMDG Class	3
	IMDG Subrisk	Not Applicable
Packing group	II	
Environmental hazard	Not Applicable	
Special precautions for user	EMS Number	F-E, S-D
	Special provisions	Not Applicable
	Limited Quantities	1 L

Transport in bulk according to Annex II of MARPOL and the IBC code

Not Applicable

Transport in bulk in accordance with MARPOL Annex V and the IMSBC Code

Product name	Group
acetonitrile	Not Available
Ecgonine Methyl Ester-D3	Not Available

Transport in bulk in accordance with the IGC Code

Product name	Ship Type
acetonitrile	Not Available
Ecgonine Methyl Ester-D3	Not Available

SECTION 15 Regulatory information

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

acetonitrile is found on the following regulatory lists

Australia Hazardous Chemical Information System (HCIS) - Hazardous Chemicals

Australian Inventory of Industrial Chemicals (AIIC)

Ecgonine Methyl Ester-D3 is found on the following regulatory lists

Australia Standard for the Uniform Scheduling of Medicines and Poisons (SUSMP) - Schedule 9

National Inventory Status

Continued...

Ecgonine Methyl Ester-D3

National Inventory	Status
Australia - AIIC / Australia Non-Industrial Use	No (Ecgonine Methyl Ester-D3)
Canada - DSL	No (Ecgonine Methyl Ester-D3)
Canada - NDSL	No (acetoneitrile; Ecgonine Methyl Ester-D3)
China - IECSC	No (Ecgonine Methyl Ester-D3)
Europe - EINEC / ELINCS / NLP	No (Ecgonine Methyl Ester-D3)
Japan - ENCS	No (Ecgonine Methyl Ester-D3)
Korea - KECI	No (Ecgonine Methyl Ester-D3)
New Zealand - NZIoC	No (Ecgonine Methyl Ester-D3)
Philippines - PICCS	No (Ecgonine Methyl Ester-D3)
USA - TSCA	No (Ecgonine Methyl Ester-D3)
Taiwan - TCSI	No (Ecgonine Methyl Ester-D3)
Mexico - INSQ	No (Ecgonine Methyl Ester-D3)
Vietnam - NCI	No (Ecgonine Methyl Ester-D3)
Russia - FBEPH	No (Ecgonine Methyl Ester-D3)
Legend:	Yes = All CAS declared ingredients are on the inventory No = One or more of the CAS listed ingredients are not on the inventory. These ingredients may be exempt or will require registration.

SECTION 16 Other information

Revision Date	07/07/2023
Initial Date	12/12/2017

SDS Version Summary

Version	Date of Update	Sections Updated
2.4	07/07/2023	Toxicological information - Acute Health (inhaled), Toxicological information - Acute Health (skin), Toxicological information - Acute Health (swallowed), Toxicological information - Chronic Health, Hazards identification - Classification, Ecological Information - Environmental, Exposure controls / personal protection - Exposure Standard, Firefighting measures - Fire Fighter (fire/explosion hazard), Firefighting measures - Fire Fighter (fire fighting), First Aid measures - First Aid (eye), First Aid measures - First Aid (inhaled), First Aid measures - First Aid (skin), Exposure controls / personal protection - Personal Protection (Respirator), Accidental release measures - Spills (major), Accidental release measures - Spills (minor), Identification of the substance / mixture and of the company / undertaking - Use

Other information

Classification of the preparation and its individual components has drawn on official and authoritative sources as well as independent review by the Chemwatch Classification committee using available literature references.

The SDS is a Hazard Communication tool and should be used to assist in the Risk Assessment. Many factors determine whether the reported Hazards are Risks in the workplace or other settings. Risks may be determined by reference to Exposures Scenarios. Scale of use, frequency of use and current or available engineering controls must be considered.

Definitions and abbreviations

PC - TWA: Permissible Concentration-Time Weighted Average
 PC - STEL: Permissible Concentration-Short Term Exposure Limit
 IARC: International Agency for Research on Cancer
 ACGIH: American Conference of Governmental Industrial Hygienists
 STEL: Short Term Exposure Limit
 TEEL: Temporary Emergency Exposure Limit,
 IDLH: Immediately Dangerous to Life or Health Concentrations
 ES: Exposure Standard
 OSF: Odour Safety Factor
 NOAEL :No Observed Adverse Effect Level
 LOAEL: Lowest Observed Adverse Effect Level
 TLV: Threshold Limit Value
 LOD: Limit Of Detection
 OTV: Odour Threshold Value
 BCF: BioConcentration Factors
 BEI: Biological Exposure Index
 AIIC: Australian Inventory of Industrial Chemicals
 DSL: Domestic Substances List
 NDSL: Non-Domestic Substances List
 IECSC: Inventory of Existing Chemical Substance in China
 EINECS: European Inventory of Existing Commercial chemical Substances
 ELINCS: European List of Notified Chemical Substances
 NLP: No-Longer Polymers
 ENCS: Existing and New Chemical Substances Inventory
 KECI: Korea Existing Chemicals Inventory
 NZIoC: New Zealand Inventory of Chemicals
 PICCS: Philippine Inventory of Chemicals and Chemical Substances
 TSCA: Toxic Substances Control Act
 TCSI: Taiwan Chemical Substance Inventory
 INSQ: Inventario Nacional de Sustancias Químicas
 NCI: National Chemical Inventory
 FBEPH: Russian Register of Potentially Hazardous Chemical and Biological Substances

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