



SAFETY DATA SHEET

Muscone

According to the REACH etc. (Amendment etc.) (EU Exit) Regulations 2020 No. 1577, as amended.

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

1.1. Product identifier

Product name	Muscone
Synonyms; trade names	musk ketone; 3,5-dinitro-2,6-dimethyl-4-tert-butylacetophenone; 4'-tert-butyl-2',6'-dimethyl-3',5'-dinitroacetophenone
CAS number	81-14-1
EU index number	609-069-00-7
EC number	201-328-9

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

Identified uses	Research and development.
Uses advised against	Not suitable for human consumption or veterinary purposes.

1.3. Details of the supplier of the safety data sheet

Supplier	Molekula Ltd. Lingfield Way, Darlington, DL1 4XX, United Kingdom +44 (0) 3302000333 info@molekula.com
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1.4. Emergency telephone number

+44 (0) 7769276927

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification (SI 2019 No. 720)

Physical hazards	Not Classified
Health hazards	Carc. 2 - H351
Environmental hazards	Aquatic Acute 1 - H400 Aquatic Chronic 1 - H410

2.2. Label elements

EC number	201-328-9
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Hazard pictograms



Signal word	Warning
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Hazard statements	H351 Suspected of causing cancer. H410 Very toxic to aquatic life with long lasting effects.
Precautionary statements	P273 Avoid release to the environment. P280 Wear protective gloves/ protective clothing/ eye protection/ face protection. P308+P313 IF exposed or concerned: Get medical advice/ attention. P405 Store locked up. P501 Dispose of contents/ container in accordance with national regulations.

2.3. Other hazards

This substance is not classified as PBT or vPvB according to current UK criteria.

SECTION 3: Composition/information on ingredients

3.1. Substances

Product name	Muscone
EU index number	609-069-00-7
CAS number	81-14-1
EC number	201-328-9
Chemical formula	C14H18N2O5

SECTION 4: First aid measures

4.1. Description of first aid measures

General information	Get medical attention if any discomfort continues. Show this Safety Data Sheet to the medical personnel.
Inhalation	Move affected person to fresh air and keep warm and at rest in a position comfortable for breathing. Loosen tight clothing such as collar, tie or belt. Get medical attention if symptoms are severe or persist.
Ingestion	Rinse mouth thoroughly with water. Get medical advice/attention if you feel unwell. Do not induce vomiting unless under the direction of medical personnel.
Skin contact	Rinse with water.
Eye contact	Remove any contact lenses and open eyelids wide apart. Rinse with water. Get medical attention if any discomfort continues.
Protection of first aiders	First aid personnel should wear appropriate protective equipment during any rescue.

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

General information	The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
Inhalation	Prolonged or repeated exposure may cause the following adverse effects: Suspected of causing cancer.
Ingestion	Prolonged or repeated exposure may cause the following adverse effects: Suspected of causing cancer.
Skin contact	Prolonged contact may cause dryness of the skin. Prolonged or repeated exposure may cause the following adverse effects: Suspected of causing cancer.
Eye contact	May be slightly irritating to eyes.

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

Notes for the doctor	Treat symptomatically.
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SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media Extinguish with alcohol-resistant foam, carbon dioxide, dry powder or water fog. Use fire-extinguishing media suitable for the surrounding fire.

Unsuitable extinguishing media Do not use water jet as an extinguisher, as this will spread the fire.

5.2. Special hazards arising from the substance or mixture

Specific hazards None known.

Hazardous combustion products Thermal decomposition or combustion products may include the following substances: Harmful gases or vapours. Oxides of carbon. Oxides of nitrogen.

5.3. Advice for firefighters

Protective actions during firefighting Avoid breathing fire gases or vapours. Evacuate area. Keep upwind to avoid inhalation of gases, vapours, fumes and smoke. Ventilate closed spaces before entering them. Cool containers exposed to heat with water spray and remove them from the fire area if it can be done without risk. Cool containers exposed to flames with water until well after the fire is out. Avoid discharge to the aquatic environment. Control run-off water by containing and keeping it out of sewers and watercourses. If risk of water pollution occurs, notify appropriate authorities.

Special protective equipment for firefighters Wear positive-pressure self-contained breathing apparatus (SCBA) and appropriate protective clothing. Firefighter's clothing will provide a basic level of protection for chemical incidents.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Personal precautions Wear protective clothing as described in Section 8 of this safety data sheet. No action shall be taken without appropriate training or involving any personal risk. Do not touch or walk into spilled material.

6.2. Environmental precautions

Environmental precautions Avoid discharge into drains or watercourses or onto the ground. Avoid discharge to the aquatic environment.

6.3. Methods and material for containment and cleaning up

Methods for cleaning up Wear protective clothing as described in Section 8 of this safety data sheet. Clear up spills immediately and dispose of waste safely. Collect spillage with a shovel and broom, or similar and reuse, if possible. Collect and place in suitable waste disposal containers and seal securely. Flush contaminated area with plenty of water. Wash thoroughly after dealing with a spillage. Dangerous for the environment. Do not empty into drains. For waste disposal, see Section 13.

6.4. Reference to other sections

Reference to other sections For personal protection, see Section 8. See Section 11 for additional information on health hazards. See Section 12 for additional information on ecological hazards. For waste disposal, see Section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

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Usage precautions Read and follow manufacturer's recommendations. Wear protective clothing as described in Section 8 of this safety data sheet. Keep away from food, drink and animal feeding stuffs. Keep container tightly sealed when not in use. Suspected of causing cancer. Avoid discharge to the aquatic environment. Do not handle until all safety precautions have been read and understood. Do not handle broken packages without protective equipment. Do not reuse empty containers.

Advice on general occupational hygiene Wash promptly if skin becomes contaminated. Take off contaminated clothing. Wash contaminated clothing before reuse.

7.2. Conditions for safe storage, including any incompatibilities

Storage precautions Store away from incompatible materials (see Section 10). Store locked up. Keep only in the original container. Keep container tightly closed, in a cool, well ventilated place. Keep containers upright. Protect containers from damage.

Storage class Miscellaneous hazardous material storage.

7.3. Specific end use(s)

Specific end use(s) The identified uses for this product are detailed in Section 1.2.

SECTION 8: Exposure controls/Personal protection

8.1. Control parameters

8.2. Exposure controls

Protective equipment



Appropriate engineering controls Provide adequate general and local exhaust ventilation. Ensure the ventilation system is regularly maintained and tested. Good general ventilation should be adequate to control worker exposure to airborne contaminants. Observe any occupational exposure limits for the product or ingredients.

Eye/face protection Unless the assessment indicates a higher degree of protection is required, the following protection should be worn: Tight-fitting safety glasses.

Hand protection No specific hand protection recommended. Avoid contact with skin.

Other skin and body protection Wear appropriate clothing to prevent repeated or prolonged skin contact.

Hygiene measures Wash after use and before eating, smoking and using the toilet. Do not eat, drink or smoke when using this product.

Respiratory protection Ensure all respiratory protective equipment is suitable for its intended use and is 'UKCA'-marked. Check that the respirator fits tightly and the filter is changed regularly. Gas and combination filter cartridges suitable for intended use should be used. Full face mask respirators with replaceable filter cartridges suitable for intended use should be used. Half mask and quarter mask respirators with replaceable filter cartridges suitable for intended use should be used.

Environmental exposure controls Keep container tightly sealed when not in use. Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental protection legislation. In some cases, fume scrubbers, filters or engineering modifications to the process equipment will be necessary to reduce emissions to acceptable levels.

SECTION 9: Physical and chemical properties

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9.1. Information on basic physical and chemical properties

Appearance	Crystalline powder.
Colour	Yellow-white.
Odour	Not known.
Odour threshold	No information available.
pH	No information available.
Melting point	135.5°C/275.9°F
Initial boiling point and range	No information available.
Flash point	> 168°C / 334°F Method: Closed cup.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Upper/lower flammability or explosive limits	No information available.
Vapour pressure	0.001 Pa @ 25°C/77°F
Vapour density	No information available.
Relative density	1.268 g/cm ³ @ 20°C/68°F
Solubility(ies)	0.1 mg/l water @ 20°C/68°F
Partition coefficient	log Pow: 4.24 at 25°C/77°F
Auto-ignition temperature	No information available.
Decomposition Temperature	No information available.

9.2. Other information

Molecular weight	294.31
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SECTION 10: Stability and reactivity

10.1. Reactivity

Reactivity	See the other subsections of this section for further details.
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10.2. Chemical stability

Stability	Stable at normal ambient temperatures and when used as recommended. Stable under the prescribed storage conditions.
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10.3. Possibility of hazardous reactions

Possibility of hazardous reactions	No potentially hazardous reactions known.
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10.4. Conditions to avoid

Conditions to avoid	There are no known conditions that are likely to result in a hazardous situation.
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10.5. Incompatible materials

Materials to avoid	No specific material or group of materials is likely to react with the product to produce a hazardous situation. Strong oxidising agents. Strong acids. Strong alkalis.
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10.6. Hazardous decomposition products

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Hazardous decomposition products	Does not decompose when used and stored as recommended. Thermal decomposition or combustion products may include the following substances: Harmful gases or vapours. Oxides of carbon. Oxides of nitrogen.
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SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity - oral

Summary Based on available data the classification criteria are not met.

Acute toxicity - dermal

Summary Based on available data the classification criteria are not met.

Acute toxicity - inhalation

Summary Based on available data the classification criteria are not met.

Skin corrosion/irritation

Summary Based on available data the classification criteria are not met.

Serious eye damage/irritation

Summary Based on available data the classification criteria are not met.

Respiratory sensitisation

Summary Based on available data the classification criteria are not met.

Skin sensitisation

Summary Based on available data the classification criteria are not met.

Germ cell mutagenicity

Summary Based on available data the classification criteria are not met.

Carcinogenicity

Summary Suspected of causing cancer.

IARC carcinogenicity

None of the ingredients are listed or exempt.

Reproductive toxicity

Summary Based on available data the classification criteria are not met.

Specific target organ toxicity - single exposure

Summary Based on available data the classification criteria are not met.

Specific target organ toxicity - repeated exposure

Summary Based on available data the classification criteria are not met.

Aspiration hazard

Summary Not relevant. Solid.

General information

May cause cancer after repeated exposure. Risk of cancer depends on duration and level of exposure. The severity of the symptoms described will vary dependent on the concentration and the length of exposure.

Inhalation

A single exposure may cause the following adverse effects: Temporary irritation.

Ingestion

May cause discomfort if swallowed.

Skin contact

Prolonged contact may cause dryness of the skin.

Eye contact

May be slightly irritating to eyes.

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Route of exposure Ingestion Inhalation Skin and/or eye contact

Target organs No specific target organs known.

SECTION 12: Ecological information

12.1. Toxicity

Acute aquatic toxicity

Summary Very toxic to aquatic life.

LE(C)₅₀ $0.1 < L(E)C_{50} \leq 1$

Acute toxicity - aquatic invertebrates EC₅₀, 48 hours: 0.46 mg/l, Daphnia magna

Acute toxicity - aquatic plants EC₅₀, 72 hours: 0.24 mg/l, Pseudokirchneriella subcapitata
NOEC, 72 hours: 0.088 mg/l, Pseudokirchneriella subcapitata

Chronic aquatic toxicity

Summary Very toxic to aquatic life with long lasting effects.

12.2. Persistence and degradability

Persistence and degradability The degradability of the product is not known.

12.3. Bioaccumulative potential

Bioaccumulative potential 47 µg/l, for 21 days BCF: 1380, Oncorhynchus mykiss (Rainbow trout)

Partition coefficient log Pow: 4.24 at 25°C/77°F

12.4. Mobility in soil

Mobility No data available.

12.5. Results of PBT and vPvB assessment

Results of PBT and vPvB assessment This product does not contain any substances classified as PBT or vPvB.

12.6. Other adverse effects

Other adverse effects None known.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

General information The generation of waste should be minimised or avoided wherever possible. Reuse or recycle products wherever possible. This material and its container must be disposed of in a safe way. When handling waste, the safety precautions applying to handling of the product should be considered. Care should be taken when handling emptied containers that have not been thoroughly cleaned or rinsed out. Empty containers or liners may retain some product residues and hence be potentially hazardous.

Disposal methods Do not empty into drains. Dispose of surplus products and those that cannot be recycled via a licensed waste disposal contractor. Waste, residues, empty containers, discarded work clothes and contaminated cleaning materials should be collected in designated containers, labelled with their contents. Incineration or landfill should only be considered when recycling is not feasible.

SECTION 14: Transport information

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General For limited quantity packaging/limited load information, consult the relevant modal documentation using the data shown in this section.

14.1. UN number

UN No. (ADR/RID)	3077
UN No. (IMDG)	3077
UN No. (ICAO)	3077
UN No. (ADN)	3077

14.2. UN proper shipping name

Proper shipping name (ADR/RID)	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (Muscone)
Proper shipping name (IMDG)	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (Muscone)
Proper shipping name (ICAO)	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (Muscone)
Proper shipping name (ADN)	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (Muscone)

14.3. Transport hazard class(es)

ADR/RID class	9
ADR/RID classification code	M7
ADR/RID label	9
IMDG class	9
ICAO class/division	9
ADN class	9

Transport labels



14.4. Packing group

ADR/RID packing group	III
IMDG packing group	III
ICAO packing group	III
ADN packing group	III

14.5. Environmental hazards

Environmentally hazardous substance/marine pollutant



14.6. Special precautions for user

Always transport in closed containers that are upright and secure. Ensure that persons transporting the product know what to do in the event of an accident or spillage.

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ADR transport category	3
Emergency Action Code	2Z
Hazard Identification Number (ADR/RID)	90
Tunnel restriction code	(-)

14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code Not applicable.

SECTION 15: Regulatory information

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

National regulations Health and Safety at Work etc. Act 1974 (as amended).
The Carriage of Dangerous Goods and Use of Transportable Pressure Equipment Regulations 2009 (SI 2009 No. 1348) (as amended) ["CDG 2009"].
EH40/2005 Workplace exposure limits.

15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

Inventories

EU - EINECS/ELINCS

None of the ingredients are listed or exempt.

SECTION 16: Other information

Abbreviations and acronyms used in the safety data sheet	ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road. ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways. RID: European Agreement concerning the International Carriage of Dangerous Goods by Rail. IATA: International Air Transport Association. ICAO: Technical Instructions for the Safe Transport of Dangerous Goods by Air. IMDG: International Maritime Dangerous Goods. CAS: Chemical Abstracts Service. ATE: Acute Toxicity Estimate. LC50: Lethal Concentration to 50 % of a test population. LD50: Lethal Dose to 50% of a test population (Median Lethal Dose). EC ₅₀ : 50% of maximal Effective Concentration. PBT: Persistent, Bioaccumulative and Toxic substance. vPvB: Very Persistent and Very Bioaccumulative.
Classification abbreviations and acronyms	Carc. = Carcinogenicity Aquatic Acute = Hazardous to the aquatic environment (acute) Aquatic Chronic = Hazardous to the aquatic environment (chronic)
Classification procedures according to SI 2019 No. 720	Carc. 2 - H351: : Expert judgement. Aquatic Acute 1 - H400: Aquatic Chronic 1 - H410: : Expert judgement.
Training advice	Only trained personnel should use this material.
Revision date	01/09/2022
Revision	1

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SDS number	1424
Hazard statements in full	H351 Suspected of causing cancer. H400 Very toxic to aquatic life. H410 Very toxic to aquatic life with long lasting effects.

This information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process. Such information is, to the best of the company's knowledge and belief, accurate and reliable as of the date indicated. However, no warranty, guarantee or representation is made to its accuracy, reliability or completeness. It is the user's responsibility to satisfy himself as to the suitability of such information for his own particular use.